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FILE COVERS 1907 - 18 Mar 2009 VOL 150 ISS 12
 FILE LAST UPDATED: 17 Mar 2009 (20090317/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L53

L41	178	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	GEBHARDT J?/AU
L42	57	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	GOTZ N?/AU
L43	43	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	JAEDICKE H?/AU
L44	1001	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	MAYER G?/AU
L45	210	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	RACK M?/AU
L52	32	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	(L41 OR L42 OR L43 OR L44 OR L45) AND ?PYRIDIN?/AB
L53	2	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	L52 AND ?PHOSPH?/AB

=> d stat que L57

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L42	57	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	GOTZ N?/AU
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L45	210	SEA FILE=CAPLUS	SPE=ON	ABB=ON	PLU=ON	RACK M?/AU
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10/584354

L57 8 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON (L54 OR L55 OR L56)

=> s L53 or L57

L60 9 L53 OR L57

=> file medline embase biosis wpix

FILE 'MEDLINE' ENTERED AT 10:36:16 ON 18 MAR 2009

FILE 'EMBASE' ENTERED AT 10:36:16 ON 18 MAR 2009

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=> d stat que L58

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L42 57 SEA FILE=CAPLUS SPE=ON ABB=ON PLU=ON GOTZ N?/AU
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L61 25 L58 OR L59

=> dup rem L60 L61

FILE 'CAPLUS' ENTERED AT 10:36:39 ON 18 MAR 2009

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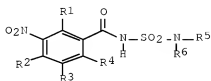
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PROCESSING COMPLETED FOR L60
PROCESSING COMPLETED FOR L61
L62 25 DUP REM L60 L61 (9 DUPLICATES REMOVED)
ANSWERS '1-9' FROM FILE CAPLUS
ANSWERS '10-17' FROM FILE BIOSIS
ANSWERS '18-25' FROM FILE WPIX

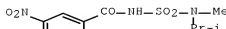
=> d ibib abs hitind L62 1-9; d iall L62 10-17; d iall hit L62 18-25

L62 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2007:619920 CAPLUS Full-text
DOCUMENT NUMBER: 147:52713
TITLE: Preparation of N-benzoylsulfamides
INVENTOR(S): Schmidt, Thomas; Gebhardt, Joachim; Loeher, Sandra;
Keil, Michael; Wevers, Jan Hendrik; Rack, Michael;
Mayer, Guido; Pleschke, Axel
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 58pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007063028	A2	20070607	WO 2006-EP68832	20061123
WO 2007063028	A3	20070823		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
DE 102005057681	A1	20070606	DE 2005-102005057681	20051201
AU 2006319263	A1	20070607	AU 2006-319263	20061123
CA 2631113	A1	20070607	CA 2006-2631113	20061123
EP 1957443	A2	20080820	EP 2006-830101	20061123
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR MX 2008006749 A 20080602 MX 2008-6749 20080526 IN 2008KN02462 A 20090123 IN 2008-KN2462 20080618 KR 2008072093 A 20080805 KR 2008-715883 20080630 CN 101351443 A 20090121 CN 2006-80050207 20080701				
PRIORITY APPLN. INFO.:			DE 2005-102005057681A	20051201

OTHER SOURCE(S): MARPAT 147:52713
GI

I



II

AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; R5, R6 = H, alkyl, alkenyl, etc.] were prepared For example, N-acylation of N-isopropyl-N-methylsulfamide with 4-fluoro-3-nitrobenzoyl chloride afforded sulfonamide II in 87% yield.

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 21

L62 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2005:612313 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:133285

TITLE: Process for the preparation of pyridine derivatives having an electron withdrawing substituent in the position 4 of the ring, particularly 4-trifluoromethylpyridines

INVENTOR(S): Gebhardt, Joachim; Goetz, Norbert; Jaedicke, Hagen; Mayer, Guido; Rack, Michael

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

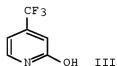
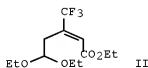
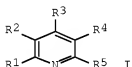
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063780	A1	20050714	WO 2004-EP14590	20041222
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004309054	A1	20050714	AU 2004-309054	20041222
CA 2550693	A1	20050714	CA 2004-2550693	20041222
EP 1723156	A1	20061122	EP 2004-804186	20041222
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,			

IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

CN 1898255	A	20070117	CN 2004-80038884	20041222
BR 2004018047	A	20070417	BR 2004-18047	20041222
JP 2007519625	T	20070719	JP 2006-546051	20041222
IN 2006DN03604	A	20070824	IN 2006-DN3604	20060622
MX 2006007401	A	20060913	MX 2006-7401	20060623
KR 2006128896	A	20061214	KR 2006-712653	20060623
US 20070249837	A1	20071025	US 2007-584354	20070604

PRIORITY APPLN. INFO.: EP 2003-29730 A 20031223
US 2003-531614P P 20031223
WO 2004-EP14590 W 20041222

OTHER SOURCE(S): CASREACT 143:133285; MARPAT 143:133285
GI



AB The invention is directed to a process for the preparation of substituted pyridine derivs. having an electron withdrawing substituent in the position 4 of the ring I [R1, R2 = independently H, (un)substituted alkyl, aryl; R3 = CN, NO2, CF3, etc.; R4 = H, (un)substituted S-alkyl, alkyl; R5 = OH, NH2] by condensation of an α - β -unsatd. carbonyl compound R3-C(O)-C(R1):C(R2)-G [R1-R3 = defined as above; G = NH2, or a leaving group] with a Wittig reagent or Horner-Wadsworth-Emmons reagent in the presence of a base, optionally followed by cyclization. For example, condensation of 4-ethoxy-1,1,1-trifluorobut-3-en-2-one with phosphonoacetic acid tri-Et ester in the presence of EtONa in EtOH, and subsequent cyclization of II with NH4OAc at 150-155 for 8 h gave pyridine III.

IC ICM C07F009-40
ICS C07C321-08; C07D213-64; C07D213-71

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2000:351514 CAPLUS Full-text

DOCUMENT NUMBER: 132:347556

TITLE: Preparation of

INVENTOR(S): 2-alkyl-3-(4,5-dihydroisoxazol-3-yl)halobenzenes.
Rack, Michael; Gotz, Norbert; Hagen, Helmut; Von
Deyn, Wolfgang; Baumann, Ernst; Lochtman, Rene;
Gebhardt, Joachim

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

10/584354

SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000029395	A1	20000525	WO 1999-EP8844	19991117
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2351466	A1	20000525	CA 1999-2351466	19991117
EP 1131307	A1	20010912	EP 1999-960983	19991117
EP 1131307	B1	20040825		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
HU 2001004190	A2	20020328	HU 2001-4190	19991117
HU 2001004190	A3	20021228		
JP 2002530275	T	20020917	JP 2000-582382	19991117
AT 274501	T	20040915	AT 1999-960983	19991117
ES 2226475	T3	20050316	ES 1999-960983	19991117
IL 143254	A	20061231	IL 1999-143254	19991117
US 6548677	B1	20030415	US 2001-856037	20010517
MX 2001004998	A	20011203	MX 2001-4998	20010518
US 20020156290	A1	20021024	US 2002-141236	20020509
US 6603017	B2	20030805		
US 20030229232	A1	20031211	US 2003-462903	20030618
US 6716989	B2	20040406		
PRIORITY APPLN. INFO.:			DE 1998-19853039	A 19981118
			WO 1999-EP8844	W 19991117
			US 2001-856037	A3 20010517
			US 2002-141236	A3 20020509
OTHER SOURCE(S):			CASREACT 132:347556; MARPAT 132:347556	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. (I; n = 0,1,2; R1, R2 = alkyl; R3, R4, R5 = H, alkyl; R4R5 = bond; R6 = Cl, Br), were prepared by (1) halogenation of 1,2-dialkylbenzenes using halogens to give 1,2-dialkyl-3,6-dihalobenzenes (II; R1 = alkyl; R6 = halo), (2) treatment of II with H2O2 and a halogenating agent, preferably HBr to give benzyl halides (III), (3) oxidation of the latter to give aldehydes (IV), (4) treatment of the latter with NH2OH and base to give oximes (V), (5) reaction of V with R3R4C:CHR5 to give isoxazoles (VI), (6) treatment of the latter with R2S-M+, and (7) optional oxidation of the thioether. Thus, 3,6-dibromo-2-methylbenzaloxime (preparation given) was pressured with ethylene and NaOCl in CH2Cl2 followed by stirring overnight to give 95% 3-(3,6-dibromo-2-methylphenyl)-4,5-dihydroisoxazole. This was heated with NaSMe in NMP at 100° to give 52.3% 3-(3-bromo-2-methyl-6-methylthiophenyl)-4,5-dihydroisoxazole.

10/584354

IC ICM C07D261-04

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2001:48787 CAPLUS Full-text

DOCUMENT NUMBER: 135:87114

TITLE: Placebo-controlled, randomized, evaluator-blinded
endoscopy study of risedronate vs. aspirin in healthy
postmenopausal women

AUTHOR(S): Lanza, F. L.; Rack, M. F.; Li, Z.; Krajewski, S. A.;
Blank, M. A.

CORPORATE SOURCE: Houston Center for Clinical Research, Houston, TX, USA

SOURCE: Alimentary Pharmacology and Therapeutics (2000),
14(12), 1663-1670

CODEN: APTHEN; ISSN: 0269-2813

PUBLISHER: Blackwell Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Bisphosphonates are effective treatments for osteoporosis. Since some primary
amino bisphosphonates are associated with esophageal injury, we conducted a
study of the upper gastrointestinal effects of risedronate, a pyridinyl
bisphosphonate. Healthy, postmenopausal women received risedronate 5 mg (n =
26), aspirin 2600 mg (n = 27), or placebo (n = 27) daily for 14 days and
underwent endoscopy at baseline. Day 8 and Day 15. Esophageal erosions were
noted in one subject in the aspirin group, two in the placebo group, and none
in the risedronate group, and an ulcer in one aspirin-treated subject.
Gastric erosions and ulcers were observed most frequently in the aspirin
group. Gastric ulcers were noted in eight subjects in the aspirin group, one
in the placebo group, and none in the risedronate group (P = 0.010, placebo
vs. aspirin; P = 0.002, risedronate vs. aspirin). Duodenal erosions and
ulcers were observed in the aspirin group only. Gastroduodenal erosion scores
of three or more occurred more frequently in the aspirin than in the
risedronate and placebo groups (P < 0.001). Risedronate 5 mg was not
associated with esophageal or gastroduodenal ulcers in healthy, post-
menopausal women, a population representative of patients who will receive
risedronate in the clin. setting.

CC 1-12 (Pharmacology)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 1999:736669 CAPLUS Full-text

DOCUMENT NUMBER: 131:351318

TITLE: Preparation of 3-isoxazolinyl-substituted acylbenzenes
INVENTOR(S): Rheinheimer, Joachim; Von Deyn, Wolfgang; Gebhardt,
Joachim; Rack, Michael; Lochtmann, Rene; Gotz,
Norbert; Keil, Michael; Witschel, Matthias; Hagen,
Helmut; Misslitz, Ulf; Baumann, Ernst

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

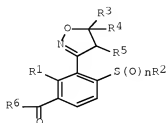
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19820722	C1	19991104	DE 1998-19820722	19980511
DE 19852095	A1	20000518	DE 1998-19852095	19981112
CA 2331816	A1	19991118	CA 1999-2331816	19990504
AU 9939305	A	19991129	AU 1999-39305	19990504
AU 772781	B2	20040506		
BR 9910326	A	20010130	BR 1999-10326	19990504
EP 1077955	A1	20010228	EP 1999-922160	19990504
EP 1077955	B1	20070627		
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HU 2001002843	A2	20020328	HU 2001-2843	19990504
HU 2001002843	A3	20040301		
JP 2002514630	T	20020521	JP 2000-548313	19990504
NZ 508648	A	20030926	NZ 1999-508648	19990504
IL 139277	A	20060312	IL 1999-139277	19990504
WO 2000029394	A1	20000525	WO 1999-EP8746	19991112
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1129082	A1	20010905	EP 1999-959276	19991112
EP 1129082	B1	20040929		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002529540	T	20020910	JP 2000-582381	19991112
AT 277915	T	20041015	AT 1999-959276	19991112
US 6525204	B1	20030225	US 2000-674535	20001102
NO 2000005652	A	20001109	NO 2000-5652	20001109
NO 318079	B1	20050131		
MX 2000011047	A	20010930	MX 2000-11047	20001110
IN 2000CN00738	A	20070511	IN 2000-CN738	20001128
US 6469176	B1	20021022	US 2001-831400	20010509
US 20030018200	A1	20030123	US 2002-180608	20020627
US 6608209	B2	20030819		
US 20030028033	A1	20030206	US 2002-223019	20020819
US 6670482	B2	20031230		
US 20030220505	A1	20031127	US 2003-436739	20030514
US 6706886	B2	20040316		
IN 2005CN03617	A	20070914	IN 2005-CN3617	20051230
US 20070161800	A1	20070712	US 2007-684630	20070311
PRIORITY APPLN. INFO.:			DE 1998-19820722	A 19980511
			DE 1998-19852095	A 19981112
			WO 1999-EP3006	W 19990504
			WO 1999-EP8746	W 19991112
			US 2000-674535	A3 20001102
			IN 2000-CN738	A3 20001128
			US 2001-831400	A3 20010509
			US 2002-180608	A3 20020627
			US 2002-223019	A3 20020819
			US 2003-417083	A3 20030417

10/584354

OTHER SOURCE(S):
GI

MARPAT 131:351318



I

AB The title compds. [I; R1 = H, C1-6 alkyl; R2 = C1-6 alkyl; R3-R5 = H, C1-6 alkyl; R4R5 = bond; R6 = heteroring; n = 0-2], useful as chemical intermediates especially for the manufacture of agrochems., were prepared by condensation of 2,6-O2N(R1)C6H3Me with organic nitrites, cyclization of the product oximes 2,6-O2NR1C6H3CH:NOH with alkenes R3R4C:CHR5 (R3-R5 as above), NO2-group reduction in the resulting 3-isoxazolinyl nitrobenzenes, conversion of the anilines with dialkyl disulfides R2SSR2 (R2 as above), benzene ring bromination of benzene thioethers, S-oxidation of bromobenzene thioethers and catalytic carboxylation (Br substitution) with CO in the presence of alcs. R6OH (R6 as above). Also claimed were 2-isoxazolinylanilines, their intermediates and new methods for producing the intermediate products. Thus, 1-methyl-4-(3-(4,5-dihydroisoxazol-3-yl)- 2-methyl-4-methylsulfonylbenzoyl)-5-hydroxypyrazole was prepared in 6 steps as described above.

IC ICM C07D261-04

ICS C07D413-10; C07C251-40; C07C319-14

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 1998:509194 CAPLUS Full-text

DOCUMENT NUMBER: 129:136165

ORIGINAL REFERENCE NO.: 129:27841a, 27844a

TITLE: Preparation of heterocyclylbenzoylpyrazoles and related compounds as herbicides.

INVENTOR(S): Von Deyn, Wolfgang; Hill, Regina Luise; Kardorff, Uwe; Baumann, Ernst; Engel, Stefan; Mayer, Guido; Witschel, Matthias; Rack, Michael; Gotz, Norbert; Gebhardt, Joachim; Misslitz, Ulf; Walter, Helmut; Westphalen, Karl-Otto; Otten, Martina; Rheinheimer, Joachim; et al.

PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

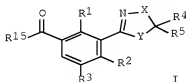
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9831681	A1	19980723	WO 1998-EP69	19980108
W: AL, AU, AZ, BG, BR, BY, CA, CN, CZ, EE, GE, HU, ID, IL, JP, KG, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, UA, US, UZ, VN, AM, MD				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2278331	A1	19980723	CA 1998-2278331	19980108
CA 2278331	C	20081118		
AU 9860929	A	19980807	AU 1998-60929	19980108
EP 958291	A1	19991124	EP 1998-905274	19980108
EP 958291	B1	20090121		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
EE 9900290	A	20000215	EE 1999-290	19980108
BR 9806778	A	20000516	BR 1998-6778	19980108
HU 2000001493	A2	20000828	HU 2000-1493	19980108
HU 2000001493	A3	20010228		
JP 2001508458	T	20010626	JP 1998-533620	19980108
NZ 336992	A	20010831	NZ 1998-336992	19980108
CN 1117750	C	20030813	CN 1998-802797	19980108
IL 130777	A	20050619	IL 1998-130777	19980108
CZ 297554	B6	20070207	CZ 1999-2523	19980108
PL 195240	B1	20070831	PL 1998-334847	19980108
SK 286069	B6	20080205	SK 1999-903	19980108
AT 421514	T	20090215	AT 1998-905274	19980108
TW 505640	B	20021011	TW 1998-87100502	19980115
ZA 9800362	A	19990716	ZA 1998-362	19980116
ZA 9800363	A	19990716	ZA 1998-363	19980116
IN 1998MA00104	A	20050304	IN 1998-MA104	19980116
NO 9903521	A	19990915	NO 1999-3521	19990716
NO 313914	B1	20021223		
BG 64232	B1	20040630	BG 1999-103658	19990810
US 20020025910	A1	20020228	US 2000-748006	20001227
US 7232792	B2	20070619		
AU 2004203481	A1	20040826	AU 2004-203481	20040729
AU 2004203481	B2	20071018		
US 20080039327	A1	20080214	US 2007-739928	20070425
PRIORITY APPLN. INFO.:			DE 1997-19701446	A 19970117
			WO 1998-EP69	W 19980108
			US 1998-91300	A1 19980616
			US 2000-748006	A3 20001227
			AU 2001-91395	A3 20011116

OTHER SOURCE(S): MARPAT 129:136165
GI



AB Title compds. [I; R1, R2 = H, NO2, halo, cyano, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl,

alkylsulfonyl, haloalkylsulfonyl; R3 = H, halo, alkyl; R4, R5 = H, halo, cyano, NO2, alkyl, alkoxyalkyl, dialkoxyalkyl, dialkylaminoalkyl, (substituted), Ph, PhCH2, etc.; R4R5 = O, S; X = O, S, NR9, CO, CR10R11; R4R9 or R4R10 or R5R12 or R5R13 = (substituted) (interrupted) alkylene; Y = O, S, NR12, CO, CR13R14; R9, R12 = H, alkyl; R10-R14 = H, alkyl, haloalkyl, alkoxycarbonyl, haloalkoxycarbonyl, CONR7R8; R15 = substituted 4-pyrazolyl, were prepared as herbicides and plant growth regulators (no data). Thus, 5-hydroxy-1-methylpyrazole in dioxane was treated with 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl chloride (preparation given) in dioxane and with Et3N in dioxane followed by 2 h stirring to give 92% 4-[2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoyl]-5-hydroxy-1-methyl-1H-pyrazole.

IC ICM C07D413-10

ICS A01N043-72; C07D498-10; C07D417-10; C07D261-04; C07D291-04;
C07D273-00; C07D263-10; C07D261-20; C07D277-10; C07D277-34;
C07D403-10; C07D419-10; C07D498-10; C07D311-00; C07D261-00

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN DUPLICATE 7

ACCESSION NUMBER: 1998:509191 CAPLUS Full-text

DOCUMENT NUMBER: 129:122657

ORIGINAL REFERENCE NO.: 129:25133a, 25136a

TITLE: Preparation of
2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-
methylsulfonylbenzoic acids and related compounds.
INVENTOR(S): Rheinheimer, Joachim; Von Deyn, Wolfgang; Gebhardt,
Joachim; Hill, Regina Luise; Rack, Michael; König,
Hartmann; Gotz, Norbert; Maywald, Volker; Kardorff,
Uwe

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

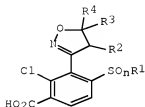
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

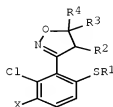
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9831676	A1	19980723	WO 1998-EP66	19980108
W: AL, AU, BG, BR, BY, CA, CN, CZ, EE, GE, HU, ID, IL, JP, KG, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, UA, US, UZ, VN, AM, AZ, MD				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9862076	A	19980807	AU 1998-62076	19980108
EP 966452	A1	19991229	EP 1998-904041	19980108
EP 966452	B1	20030502		
R: CH, DE, FR, GB, LI				
JP 2001508075	T	20010619	JP 1998-533617	19980108
TW 462965	B	20011111	TW 1998-87100495	19980115
US 6124469	A	20000926	US 1999-341519	19990713
US 20020025910	A1	20020228	US 2000-748006	20001227
US 7232792	B2	20070619		
AU 2004203481	A1	20040826	AU 2004-203481	20040729
AU 2004203481	B2	20071018		
PRIORITY APPLN. INFO.:			DE 1997-19701446	A 19970117
			DE 1997-19709118	A 19970306

WO 1998-EP66 W 19980108
 US 1998-91300 A1 19980616
 AU 2001-91395 A3 20011116

OTHER SOURCE(S): CASREACT 129:122657; MARPAT 129:122657
 GI



I



II

AB Title compds. [I; n = 0-2; R1 = alkyl, haloalkyl; R2-R4 = H, alkyl, haloalkyl; R3R4 = (alkyl-substituted) alkylene] were prepared by treatment of thioethers (II; R1-R4 as above; X = H) with a brominating agent to give II (R1-R4 as above; X = Br) followed by treatment with a Grignard reagent and CO2 followed by optional oxidation. Thus, 3-(2-chloro-6-methylthiophenyl)-4,5-dihydroisoxazole in H2SO4 was treated with Br2 to give 82.6% 3-(3-bromo-2-chloro-6-methylthiophenyl)-4,5-dihydroisoxazole. The latter in THF was treated with Me2CHMgBr and then with dry ice to give 68% 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylthiobenzoic acid. This in HOAc was treated with Na2WO4 and H2O2 to give 90.9% 2-chloro-3-(4,5-dihydroisoxazol-3-yl)-4-methylsulfonylbenzoic acid.

IC ICM C07D261-04

ICS C07D261-20

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2000:175796 CAPLUS Full-text

DOCUMENT NUMBER: 132:207770

TITLE: Preparation of oxocyclohexenylquinolines as herbicides.

INVENTOR(S): Witschel, Matthias; Misslitz, Ulf; Baumann, Ernst; Von Deyn, Wolfgang; Langemann, Klaus; Mayer, Guido; Neidlein, Ulf; Gotz, Roland; Gotz, Norbert; Rack, Michael; Engel, Stefan; Otten, Martina; Westphalen, Karl-Otto; Walter, Helmut

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000014069	A1	20000316	WO 1999-EP6322	19990827

W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR,
KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US,
VN, ZA, AM, AZ, KG, MD, TJ, TM

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE

CA 2343144	A1	20000316	CA 1999-2343144	19990827
AU 9957425	A	20000327	AU 1999-57425	19990827
EP 1112256	A1	20010704	EP 1999-944541	19990827
EP 1112256	B1	20031029		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

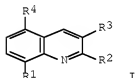
JP 2002524448	T	20020806	JP 2000-568828	19990827
US 7030063	B1	20060418	US 2001-763704	20010226

PRIORITY APPLN. INFO.:

DE 1998-19840799	A	19980908
WO 1999-EP6322	W	19990827

OTHER SOURCE(S): MARPAT 132:207770

GI



AB Title compds. [I; R1 = H, NO2, halo, cyano, alkyl, haloalkyl, alkoxyiminomethyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl, haloalkylsulfonyl, (substituted) aminosulfonyl, sulfonfylamino, PhO, heterocyclyloxy, PhS, heterocyclylthio; R2, R3 = H, alkyl, haloalkyl, halo; R4 = substituted (3-oxo-1-cyclohexen-2-yl)carbonyl, (1,3-dioxo-2-cyclohexyl)methylidene], were prepared Thus, 2-(8-chloroquinolin-5-yl)carbonyl-4,4,6,6-tetramethylcyclohexan-1,3,5-trione in CH2Cl2 was treated with (COCl)2 and DMF followed by 1.5 h stirring to give 2-[(8-chloroquinolin-5-yl)carbonyl]-1-chloro-4,4,6,6-tetramethylcyclohex-1-en-1,3,5-trione and 2-(8-chloroquinolin-5-yl)chloromethylidene-4,4,6,6-tetramethylcyclohexan-1,3,5-trione. Several I at 0.125-0.25 kg/ha postemergent showed very good activity against *Setaria faberi*, *Setaria viridis*, and *Solanum nigrum*.

IC ICM C07D215-18
ICS A01N043-42; C07D215-14; C07D215-36; C07D405-12; C07D401-08;
C07D401-06; C07F009-60

CC 27-17 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 5

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1998:485043 CAPLUS Full-text

DOCUMENT NUMBER: 129:95490

ORIGINAL REFERENCE NO.: 129:19699a,19702a

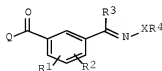
TITLE: Preparation of substituted 4-benzoylpyrazoles as herbicides.

INVENTOR(S): Hill, Regina Luise; Kardorff, Uwe; Rack, Michael;
Gotz, Norbert; Baumann, Ernst; Von Deyn, Wolfgang;
Engel, Stefan; Mayer, Guido; Otten, Martina;
Reinheimer, Joachim; Witschel, Matthias; Misslitz,

10/584354

Ulf; Walter, Helmut; Westphalen, Karl-otto
 BASF A.-G., Germany
 PATENT ASSIGNEE(S): PCT Int. Appl., 296 pp.
 SOURCE: CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9829392	A1	19980709	WO 1997-EP7210	19971219
W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ, AM, AZ, KG, MD, TJ, TM RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19700096	A1	19980709	DE 1997-19700096	19970103
CA 2276463	A1	19980709	CA 1997-2276463	19971219
CA 2276463	C	20070710		
AU 9860908	A	19980731	AU 1998-60908	19971219
AU 744201	B2	20020221		
EP 960100	A1	19991201	EP 1997-954936	19971219
EP 960100	B1	20030709		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, PT				
CN 1247532	A	20000315	CN 1997-181884	19971219
CN 1106385	C	20030423		
BR 9714257	A	20000418	BR 1997-14257	19971219
HU 2000000491	A2	20000628	HU 2000-491	19971219
HU 2000000491	A3	20011228		
JP 2001508421	T	20010626	JP 1998-529588	19971219
NZ 336452	A	20010629	NZ 1997-336452	19971219
IL 130600	A	20030112	IL 1997-130600	19971219
AT 244705	T	20030715	AT 1997-954936	19971219
PT 960100	T	20031128	PT 1997-954936	19971219
ES 2203832	T3	20040416	ES 1997-954936	19971219
SK 284921	B6	20060202	SK 1999-868	19971219
CZ 297520	B6	20070103	CZ 1999-2393	19971219
PL 193702	B1	20070330	PL 1946-3345	19971219
ZA 9800007	A	19990702	ZA 1998-7	19980102
US 6028035	A	20000222	US 1999-331671	19990623
PRIORITY APPLN. INFO.:				
		MARPAT 129:95490	DE 1997-19700096	A 19970103
			WO 1997-EP7210	W 19971219
OTHER SOURCE(S):				
GI				



I

AB Title compds. [I; R1, R2 = H, NO2, halo, cyano, rhodano, alkyl, haloalkyl, alkoxyalkyl, alkenyl, alkynyl, OR5, OCOR6, OSO2R6, SH, SONR7, SO2OR5, SO2NR5R8, NR8SO2R6, NR8COR6; R3 = H, cyano, alkyl, haloalkyl, OR7, SR7, NR7R10; R4 = H, (substituted) alkyl, cycloalkyl, alkenyl, cycloalkenyl,

alkynyl, COR9, CO2R9, COSR9 CONR8R9; X = O, NR8; n = 0, 1, 2; R5 = H, alkyl, haloalkyl, alkoxyalkyl, alkenyl, alkynyl; R6 = alkyl, haloalkyl; R7 = alkyl, haloalkyl, alkoxyalkyl, alkenyl, alkynyl; R8 = H, alkyl; R9 = alkyl, alkenyl, alkynyl, Ph, PhCH2; R10 = alkyl, haloalkyl, alkenyl, alkynyl; Q = substituted pyrazol-4-yl, were prepared as herbicides (no data). Thus, 2,4-dichloro-3-ethoxymethylbenzoic acid, 2-ethyl-3-hydroxypyrazole, and DCC were stirred 12 h in MeCN at room temperature to give 4-(2,4-dichloro-3-ethoxymethylbenzoyl)-2-ethyl-3-hydroxypyrazole.

IC ICM C07D231-20

ICS C07D231-22; C07D231-24; A01N043-56

CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 10 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on STN

ACCESSION NUMBER: 2007:426396 BIOSIS Full-text

DOCUMENT NUMBER: PREV200700425611

TITLE: 3-heterocyclyl-substituted benzoyl derivatives.

AUTHOR(S): Anonymous; von Deyn, Wolfgang [Inventor]; Hill, Regina Luise [Inventor]; Kardorff, Uwe [Inventor]; Baumann, Ernst [Inventor]; Engel, Stefan [Inventor]; Mayer, Guido [Inventor]; Witschel, Matthias [Inventor]; Rack, Michael [Inventor]; Gotz, Norbert [Inventor]; Gebhardt, Joachim [Inventor]; MiBlitz, Ulf [Inventor]; Walter, Helmut [Inventor]; Westphalen, Karl-Otto [Inventor]; Otten, Martina [Inventor]; Rheinheimer, Joachim [Inventor]

CORPORATE SOURCE: Neustadt, Germany

ASSIGNEE: BASF Aktiengesellschaft

PATENT INFORMATION: US 07232792 20070619

SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (JUN 19 2007)
CODEN: OGPUPE7. ISSN: 0098-1133.

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 8 Aug 2007

Last Updated on STN: 8 Aug 2007

ABSTRACT: Benzoyl derivatives of the formula I where the variables have the following meanings: R-1, R(2) are hydrogen, nitro, halogen, cyano, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl or C-1-C-6-haloalkylsulfonyl; R(3) is hydrogen, halogen or alkyl; R-4, R(5) are hydrogen, halogen, cyano, nitro, alkyl, alkoxy, alkylthio, dialkylamino, phenyl or carbonyl, it being possible for the 6 last-mentioned radicals to be substituted; X is O, S, NR9, CO or (CRR11)-R-10; Y is O, S, NR12, CO or (CRR14)-R-13; R(15) is pyrazole which is unsubstituted or substituted, linked in the 4-position and has attached to it in the 5-position a hydroxyl or sulfonyloxy radical; and the agriculturally useful salts thereof; processes and intermediates for the preparation of the 3-heterocyclyl-substituted benzoyl derivatives, compositions comprising them; and the use of these derivatives or compositions comprising them for controlling undesirable plants.

NAT. PATENT. CLASSIF.: 504266000

CONCEPT CODE: Pest control: general, pesticides and herbicides 54600

INDEX TERMS: Major Concepts

Methods and Techniques; Pesticides

INDEX TERMS: Chemicals & Biochemicals

3-heterocyclyl-substituted benzoyl derivative-comprising
composition: pesticide, herbicide;
3-heterocyclyl-substituted benzoyl derivatives
INDEX TERMS: Methods & Equipment
3-heterocyclyl-substituted benzoyl derivatives
preparation method: laboratory techniques
ORGANISM: Classifier
Tracheophyta 22000
Super Taxa
Plantae
Organism Name
weed (common): pest
Taxa Notes
Plants, Vascular Plants

L62 ANSWER 11 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on
STN

ACCESSION NUMBER: 2006:398397 BIOSIS Full-text
DOCUMENT NUMBER: PREV200600398711
TITLE: Cyclohexenonequinolinoyl-derivatives as herbicidal agents.
Witschel, Matthias [Inventor]; Misslitz, Ulf [Inventor];
AUTHOR(S): Baumann, Ernst [Inventor]; von Deyn, Wolfgang [Inventor];
Langemann, Klaus [Inventor]; Mayer, Guido [Inventor];
Neidlein, Ulf [Inventor]; Gotz, Roland [Inventor]; Gotz,
Norbert [Inventor]; Rack, Michael [Inventor]; Engel,
Stefan [Inventor]; Otten, Martina [Inventor]; Westphalen,
Karl-Otto [Inventor]; Walter, Helmut [Inventor]
CORPORATE SOURCE: Ludwigshafen, Germany
ASSIGNEE: BASF Aktiengesellschaft
PATENT INFORMATION: US 07030063 20060418
SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (APR 18 2006)
CODEN: OGUPE7. ISSN: 0098-1133.
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 9 Aug 2006
Last Updated on STN: 9 Aug 2006

ABSTRACT: Cyclohexenonequinolinoyl derivatives of the formula I where: R(1) is
hydrogen, nitro, halogen, cyano, alkyl, haloalkyl, alkoxyiminomethyl, alkoxy,
haloalkoxy, alkylthio, C-1-C-6-haloalkylthio, alkylsulfinyl, haloalkylsulfinyl,
alkylsulfonyl, haloalkylsulfonyl, unsubstituted or substituted amino sulfonyl,
unsubstituted or substituted sulfonyl amino, unsubstituted or substituted
phenoxy, unsubstituted or substituted heterocycloxy, unsubstituted or
substituted phenylthio or unsubstituted or substituted heterocyclylthio; R-2,
R(3) are hydrogen, alkyl, haloalkyl or halogen; R(4) is substituted
(3-oxo-1-cyclohexen-2-yl)carbonyl or substituted
(1,3-dioxo-2-cyclohexyl)methylidene; and their agriculturally useful salts;
processes for preparing the cyclohexenonequinolinoyl derivatives; compositions
comprising them, and the use of these derivatives or compositions comprising
them for controlling undesirable plants are described.

NAT. PATENT. CLASSIF.: 504247000
CONCEPT CODE: Pest control: general, pesticides and herbicides 54600
INDEX TERMS: Major Concepts
Pesticides
INDEX TERMS: Chemicals & Biochemicals
cyclohexenonequinolinoyl derivatives: pesticide,
herbicide

L62 ANSWER 12 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on
STN

10/584354

ACCESSION NUMBER: 2004:249642 BIOSIS Full-text
DOCUMENT NUMBER: PREV200400249628
TITLE: Preparation of 2-alkyl-3-(4,5-dihydroisoxazol-3-yl) halobenzenes.
AUTHOR(S): Rack, Michael [Inventor, Reprint Author]; Gotz, Norbert [Inventor]; Hagen, Helmut [Inventor]; von Deyn, Wolfgang [Inventor]; Baumann, Ernst [Inventor]; Lochtmann, Rene [Inventor]; Gebhardt, Joachim [Inventor]
CORPORATE SOURCE: Heidelberg, Germany
ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany
PATENT INFORMATION: US 6716989 20040406
SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Apr 6 2004) Vol. 1281, No. 1.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 6 May 2004
Last Updated on STN: 6 May 2004
ABSTRACT: A novel process for preparing the compounds of the formula I ##STR1## where: n is 0, 1 or 2; R1, R2 are C1 -C6 -alkyl; R3, R4, R5 are hydrogen or C1 -C6 -alkyl, or R4 and R5 together form a bond; R6 is Cl, Br, which comprises a synthesis sequence starting from 1,2-dialkylbenzenes of the formula II ##STR2## with subsequent halogenation to give 3,6-dihalo-1,2-dialkylbenzenes, haloalkylation to give benzyl bromides, oxidation to give benzaldehydes, oximation, reaction with alkenes to give isoxazoles, conversion into thioethers and, if appropriate, oxidation to give sulphenyl or sulfonyl derivatives of the formula I.
NAT. PATENT. CLASSIF.: 548240000
CONCEPT CODE: Biochemistry studies - General 10060
INDEX TERMS: Major Concepts
Biochemistry and Molecular Biophysics; Methods and Techniques
INDEX TERMS: Chemicals & Biochemicals
2-alkyl-3-(4,5-dihydroisoxazol-3-yl) halobenzenes
INDEX TERMS: Methods & Equipment
2-alkyl-3-(4,5-dihydroisoxazol-3-yl) halobenzene
preparation process: laboratory techniques
L62 ANSWER 13 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on STN
ACCESSION NUMBER: 2004:222454 BIOSIS Full-text
DOCUMENT NUMBER: PREV200400225313
TITLE: Process and novel intermediates for preparing isoxazolin-3-ylacyl benzenes.
AUTHOR(S): von Deyn, Wolfgang [Inventor, Reprint Author]; Gebhardt, Joachim [Inventor]; Rack, Michael [Inventor]; Lochtmann, Rene [Inventor]; Gotz, Norbert [Inventor]; Keil, Michael [Inventor]; Witschel, Matthias [Inventor]; Hagen, Helmut [Inventor]; Misslitz, Ulf [Inventor]; Baumann, Ernst [Inventor]
CORPORATE SOURCE: Neustadt, Germany
ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany
PATENT INFORMATION: US 6706886 20040316
SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Mar 16 2004) Vol. 1280, No. 3.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).
DOCUMENT TYPE: Patent
LANGUAGE: English

10/584354

ENTRY DATE: Entered STN: 21 Apr 2004

Last Updated on STN: 21 Apr 2004

ABSTRACT: The present invention describes a process for preparing isoxazoles of the formula I ##STR1## where: R1 is hydrogen, C1 -C6 -alkyl, R2 is hydrogen, C1 -C6 -alkyl, R3, R4, R5 are each hydrogen, C1 -C6 -alkyl or R4 and R5 together form a bond, R6 is a heterocyclic ring, n is 0, 1 or 2; which comprises preparing an intermediate of the formula VI ##STR2## where R1, R3, R4 and R5 are each as defined above, followed by halogenation, thiomethylation, oxidation and acylation to give compounds of the formula I. Furthermore, the invention describes novel intermediates for preparing the compounds of the formula I and novel processes for preparing the intermediates.

NAT. PATENT. CLASSIF.: 548240000

CONCEPT CODE: Biochemistry studies - General 10060

INDEX TERMS: Major Concepts
Biochemistry and Molecular Biophysics; Methods and Techniques

INDEX TERMS: Chemicals & Biochemicals
isoxazolin-3-ylacyl benzene intermediates;
isoxazolin-3-ylacyl benzenes

INDEX TERMS: Methods & Equipment
isoxazolin-3-ylacyl benzene intermediate preparing
process: laboratory techniques; isoxazolin-3-ylacyl
benzene preparing process: laboratory techniques

L62 ANSWER 14 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on STN

ACCESSION NUMBER: 2004:80858 BIOSIS Full-text

DOCUMENT NUMBER: PREV200400082683

TITLE: Process and novel intermediates for preparing isoxazolin-3-ylacyl benzenes.

AUTHOR(S): von Deyn, Wolfgang [Inventor, Reprint Author]; Gebhardt, Joachim [Inventor]; Rack, Michael [Inventor]; Lochtmann, Rene [Inventor]; Gotz, Norbert [Inventor]; Keil, Michael [Inventor]; Witschel, Matthias [Inventor]; Hagen, Helmut [Inventor]; Misslitz, Ulf [Inventor]; Baumann, Ernst [Inventor]

CORPORATE SOURCE: Neustadt, Germany

ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany

PATENT INFORMATION: US 6670482 20031230

SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Dec 30 2003) Vol. 1277, No. 5.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 4 Feb 2004

Last Updated on STN: 4 Feb 2004

ABSTRACT: The present invention describes a process for preparing isoxazoles of the formula I ##STR1## where: R1 is hydrogen, C1 -C6 -alkyl, R2 is hydrogen, C1 -C6 -alkyl, R3, R4, R5 are each hydrogen, C1 -C6 -alkyl or R4 and R5 together form a bond, R6 is a heterocyclic ring, n is 0, 1 or 2; which comprises preparing an intermediate of the formula VI ##STR2## where R1, R3, R4 and R5 are each as defined above, followed by halogenation, thiomethylation, oxidation and acylation to give compounds of the formula I. Furthermore, the invention describes novel intermediates for preparing the compounds of the formula I and novel processes for preparing the intermediates.

NAT. PATENT. CLASSIF.: 548240000

CONCEPT CODE: Biochemistry studies - General 10060

INDEX TERMS: Major Concepts
Biochemistry and Molecular Biophysics; Methods and

10/584354

Techniques
INDEX TERMS: Chemicals & Biochemicals
isoxazolin-3-ylacyl benzenes: novel intermediates,
process

L62 ANSWER 15 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on
STN

ACCESSION NUMBER: 2003:422051 BIOSIS Full-text
DOCUMENT NUMBER: PREV200300422051
TITLE: Preparation of isoxazolin-3-ylacylbenzenes.
AUTHOR(S): Rheinheimer, Joachim [Inventor, Reprint Author]; von Deyn,
Wolfgang [Inventor]; Gebhardt, Joachim [Inventor]; Rack,
Michael [Inventor]; Lochtmann, Rene [Inventor]; Gotz,
Norbert [Inventor]; Keil, Michael [Inventor]; Witschel,
Matthias [Inventor]; Hagen, Helmut [Inventor]; Misslitz,
Ulf [Inventor]; Baumann, Ernst [Inventor]

CORPORATE SOURCE: Ludwigshafen, Germany
ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany

PATENT INFORMATION: US 6608209 20030819
SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (Aug 19 2003) Vol. 1273, No. 3.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 10 Sep 2003
Last Updated on STN: 10 Sep 2003

ABSTRACT: A process is described for preparing isoxazoles of the formula I
##STR1## wherein R1 is hydrogen, C1 -C6 -alkyl, R2 is C1 -C6 -alkyl, R3, R4, R5
are hydrogen, C1 -C6 -alkyl, or R4 and R5 together form a bond, R6 is a
heterocyclic ring, n is 0, 1 or 2; in which an intermediate of the formula VI
##STR2## is prepared, followed by halogenation, thiomethylation, oxidation and
acylation to give compounds of formula I. Novel intermediates for preparing
the intermediates are described.
NAT. PATENT. CLASSIF.: 548240000

CONCEPT CODE: Agronomy - Miscellaneous and mixed crops 52502
Pest control: general, pesticides and herbicides 54600
Major Concepts
Agrichemicals; Methods and Techniques

INDEX TERMS: Chemicals & Biochemicals
isoxazolin-3-ylacylbenzenes: herbicide

INDEX TERMS: Methods & Equipment
isoxazolin-3-ylacylbenzene preparation: applied and
field techniques

L62 ANSWER 16 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on
STN

ACCESSION NUMBER: 2003:237403 BIOSIS Full-text
DOCUMENT NUMBER: PREV200300237403
TITLE: Method of producing
2-alkyl-3-(4,5-dihydroisoxazole-3-yl)-halobenzenes.
AUTHOR(S): Rack, Michael [Inventor, Reprint Author]; Gotz, Norbert
[Inventor]; Hagen, Helmut [Inventor]; von Deyn, Wolfgang
[Inventor]; Baumann, Ernst [Inventor]; Lochtmann, Rene
[Inventor]; Gebhardt, Joachim [Inventor]

CORPORATE SOURCE: Heidelberg, Germany
ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany

PATENT INFORMATION: US 6548677 20030415
SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (Apr 15 2003) Vol. 1269, No. 3.

<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 14 May 2003
Last Updated on STN: 14 May 2003

ABSTRACT: A novel process for preparing the compounds of the formula I ##STR1## where: n is 0, 1 or 2; R1, R2 are C1-C6 -alkyl; R3, R4, R5 are hydrogen or C1-C6 -alkyl, or R4 and R5 together form a bond; R6 is Cl, Br, which comprises a synthesis sequence starting from 1,2-dialkylbenzenes of the formula II ##STR2## with subsequent halogenation to give 3,6-dihalo-1,2-dialkylbenzenes, haloalkylation to give benzyl bromides, oxidation to give benzaldehydes, oximation, reaction with alkenes to give isoxazoles, conversion into thioethers and, if appropriate, oxidation to give sulfenyl or sulfonyl derivatives of the formula I.

NAT. PATENT. CLASSIF.: 548240000

CONCEPT CODE: Clinical biochemistry - General methods and applications
10006

INDEX TERMS: Major Concepts
Clinical Chemistry (Allied Medical Sciences); Methods
and Techniques

INDEX TERMS: Methods & Equipment
2-alkyl-3-(4,5-dihydroisoxazole-3-yl)-halobenzene
production method: laboratory techniques

L62 ANSWER 17 OF 25 BIOSIS COPYRIGHT (c) 2009 The Thomson Corporation on
STN

ACCESSION NUMBER: 2003:162079 BIOSIS Full-text

DOCUMENT NUMBER: PREV200300162079

TITLE: Method for producing isoxazoline-3-yl-acyl benzene.

AUTHOR(S): Rheinheimer, Joachim [Inventor, Reprint Author]; von Deyn, Wolfgang [Inventor]; Gebhardt, Joachim [Inventor]; Rack, Michael [Inventor]; Lochtman, Rene [Inventor]; Gotz, Norbert [Inventor]; Keil, Michael [Inventor]; Witschel, Matthias [Inventor]; Hagen, Helmut [Inventor]; Misslitz, Ulf [Inventor]; Baumann, Ernst [Inventor]

CORPORATE SOURCE: Ludwigshafen, Germany

ASSIGNEE: BASF Aktiengesellschaft, Ludwigshafen, Germany

PATENT INFORMATION: US 6525204 20030225

SOURCE: Official Gazette of the United States Patent and Trademark
Office Patents, (Feb 25 2003) Vol. 1267, No. 4.
<http://www.uspto.gov/web/menu/patdata.html>. e-file.
ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 26 Mar 2003
Last Updated on STN: 26 Mar 2003

ABSTRACT: A process is described for preparing isoxazol-3-ylacylbenzenes. Also, novel intermediates for preparing isoxazol-3-ylacylbenzenes and novel processes for preparing the intermediates are described.

NAT. PATENT. CLASSIF.: 548240000

CONCEPT CODE: Agronomy - Miscellaneous and mixed crops 52502
Pest control: general, pesticides and herbicides 54600

INDEX TERMS: Major Concepts
Agrichemicals; Methods and Techniques

INDEX TERMS: Chemicals & Biochemicals
isoxazoline-3-yl-acyl benzene: herbicide

INDEX TERMS: Methods & Equipment
isoxazoline-3-yl-acyl benzene production: laboratory
techniques

L62 ANSWER 18 OF 25 WPIX COPYRIGHT 2009 THOMSON REUTERS on STN
 ACCESSION NUMBER: 2008-019388 [82] WPIX Full-text
 DOC. NO. CPI: C2008-455885 [82]
 TITLE: Combating pest, comprises contacting the pest or their
 food supply, habitat, breeding ground or their locus with
 new or known 3-pyridyl compounds
 C01; C02
 DERWENT CLASS:
 INVENTOR: ANSPAUGH D D; BREUNINGER D; CULBERTSON D L; KUHN D G;
 FARRA RAPADO L; PUHL M; RACK M
 PATENT ASSIGNEE:
 COUNTRY COUNT: (BADI-C) BASF SE
 120

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2008065145	A1	20080605	(200882)*	EN	127[0]	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2008065145	A1	WO 2007-EP62961	20071128

PRIORITY APPLN. INFO: US 2006-867642P 20061129

INT. PATENT CLASSIF.:

IPC ORIGINAL: A01N0043-34 [I,C]; A01N0043-40 [I,A]; A01N0043-48 [I,C];
 A01N0043-50 [I,A]; A01N0043-56 [I,A]; A01N0043-72 [I,C];
 A01N0043-78 [I,A]; A01N0043-80 [I,A]; A01P0007-04 [I,A];
 A01P0007-04 [I,C]

BASIC ABSTRACT:

WO 2008065145 A1 UPAB: 20081222

NOVELTY - Combating pest, comprises contacting the pest or their food supply, habitat, breeding ground or their locus with 3-pyridyl compounds (I) and their salts.

DETAILED DESCRIPTION - Combating pest, comprises contacting the pest or their food supply, habitat, breeding ground or their locus with 3-pyridyl compounds of formula (I) and their salts.

A = e.g. chemical bond or CH₂;

X = chemical bond or 1-3C-alkylene;

y = 0 or 1;

n = 0-2;

R₁, R₂ = e.g. H, halo or CN;R₃ = H, halo or 1-6C-alkyl;R₄ = H or 1-6C-alkyl;R₅ = halo, OH, CN or 1-6C-(halo)alkyl;R₆ = e.g. 1-10C-alkyl, 2-10C-alkenyl or 2-10C-alkynyl.

Full Definitions are given in the DEFINITIONS (Full Definitions) Field.

INDEPENDENT CLAIMS are included for:

(1) a method for protecting growing plants from attack or infestation by pests comprising applying to the plant, or to the soil or artificial substrate or the water in which the plant is growing, (I);

(2) seed, comprising (I) and/or their N-oxide or salts;

(3) new 3-pyridyl compounds (I) (provided that: X-R₆ is not CH₃; and (I) and their salts excludes (I) (where R₁ is fluoro, R₂-R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is imidazolidin-

2,3-dion-1-ylmethyl (succinimidylmethyl), phthalimid-1-yl, 2-oxo-tetrahydrofuran-4-yl, 2-oxo-2,5-dihydrofuran-4-yl, N-(2-hydroxybenzoyl)aminomethyl, 5,5-dimethyl-3-oxocyclohexenyl, 3-oxocyclohexenyl, 2,2-bis(ethoxycarbonyl)ethenyl, ethyl, n-propyl, n-butyl, 2-propyl, n-pentyl, 2-methylpropan-1-yl, 3,3-dimethylpropin-3-yl and 1,1-dimethylpropan-1-yl), (I) (where R2 is fluoro, R1, R3 and R4 are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R6 is n-propyl), (I) (where R1 is chloro, R2-R4 are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R6 is ethyl, 3,3-dimethylpropin-3-yl or 1,1-dimethylpropan-1-yl), (I) (where R1 is methyl, R2-R4 are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R6 is ethyl), (I) (where R1 is chloro, R2 is methyl, R3, R4 are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R6 is n-pentyl, 1,1-dimethylpropan-1-yl or 3,3-dimethylpropin-3-yl), (I) (where R1-R4 are hydrogen, A is CH2, y and n are zero, and the moiety X-R6 is ethyl, 3-propenyl (allyl), 3-hydroxypropen-1-yl, 3-fluoropropan-1-yl or 3-(methylsulfonyloxy)propan-1-yl), (I) (where R2 is bromo, R1, R3, R4 are hydrogen, A is CH2, y and n are zero, and the moiety X-R6 is 3-propenyl), and (I) (where R1 is chloro, R2-R4 are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R6 is 3-amino-4-((2-chloropyridin-5-yl)oxy)butyl)); and

(4) synergistic pesticidal mixtures, comprising (I), and a pesticide comprising organo(thio)phosphates, carbamates, pyrethroids, growth regulators, neonicotinoids, nicotinic receptor agonists/antagonists compounds, gamma amino butyric acid antagonist compounds, macrocyclic lactone insecticides, mitochondrial electron transport inhibitor I-III compounds, oxidative phosphorylation inhibitor compounds, molting disruptor compounds, mixed function oxidase inhibitor compounds, sodium channel blocker compounds, bencloraz, bifentaz, cartap, flonicamid, pyridalyl, pymetrozine, sulfur, thiocyclam, flubendiamide, cyenopyrafen, flupyrzofos, cyflumetofen, amdiflumet, hydrazone compounds of formula N-R1aa-2,2-dihalo-1-R1bb-cyclopropanecarboxamide-2-(2,6-dichloro- a, a, a-tri-fluoro-p-tolyl)hydrazone or N-R1aa-2,2-di(R1cc)propionamide-2-(2,6-dichloro- a, a, a-trifluoro-p-tolyl)-hydrazone, or an anthranilamide compound of formula (III).

R1aa, R1cc = CH3 or ethyl;

halo = chloro or bromo;

R1bb = H or CH3;

A1 = CH3, Cl, Br or I;

X = C-H, C-Cl, C-F or N;

Y1a = F, Cl or Br;

Y1b = F, Cl or CF3;

B1 = H, Cl, Br, I or CN;

B2 = Cl, Br, CF3, OCH2CF3 or OCF2H; and

R1B = H, CH3 or CH(CH3)2.

ACTIVITY - Pesticide; Insecticide; Arthropodicide; Nematocide;

Arachnidicide.

MECHANISM OF ACTION - None given.

USE - (I) are useful for: combating pests; protecting seed; and protecting growing plants from attack or infestation by pests, which are e.g. insects (claimed), arthropods, nematodes and arachnids. (I) are useful for protecting materials against infestation and/or destruction by the pests. The ability of (I) to combat pest was tested against Aphis gossypii. The result showed that 3-chloro-5-((S)-1-phenyl-azetidin-2-ylmethoxy)-pyridine showed over 90% mortality in comparison with untreated controls, at 300 ppm.

ADVANTAGE - (I) in combination with pesticide exhibit synergistic effect (claimed). (I) are efficient to combat pest, in particular arthropod pests and nematode pest. MANUAL CODE: CPI: C05-B01B; C05-C06; C06-H; C07-H; C10-A08; C10-A10;

C10-A19; C10-B02F; C14-B01; C14-B04; C14-D05A; C14-L01;
C14-L06; C14-S09; C14-S18

IN ANSPAUGH D D; BREUNINGER D; CULBERTSON D L; KUHN D G; PARRA RAPADO L; PUHL

M; RACK M

DETD DETAILED DESCRIPTION - Combating pest, comprises contacting the pest or their food supply, habitat, breeding ground or their locus with 3-pyridyl compounds of formula (I) and their salts.

A = e.g. chemical bond or CH₂;

X = chemical bond or 1-3C-alkylene;

y = 0 or 1;

n = 0-2;

R₁, R₂ = e.g. H, halo or CN;

R₃ = H, halo or 1-6C-alkyl;

R₄ = H or 1-6C-alkyl;

R₅ = halo, OH, CN or 1-6C-(halo)alkyl;

R₆ = e.g. 1-10C-alkyl, 2-10C-alkenyl or 2-10C-alkynyl.

Full Definitions are given in the DEFINITIONS (Full Definitions)

Field. INDEPENDENT CLAIMS are included for:

(1) a method for protecting growing plants from attack or infestation by pests comprising applying to the plant, or to the soil or artificial substrate or the water in which the plant is growing, (I);

(2) seed, comprising (I) and/or their N-oxide or salts;

(3) new 3-pyridyl compounds (I) (provided that: X-R₆ is not CH₃; and (I) and their salts are excluded (I) (where R₁ is fluoro, R₂-R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is imidazolidin-2,3-dion-1-ylmethyl (succinimidylmethyl), phthalimid-1-yl, 2-oxo-tetrahydrofuran-4-yl, 2-oxo-2,5-dihydrofuran-4-yl, N-(2-hydroxybenzoyl)aminomethyl, 5,5-dimethyl-3-oxocyclohexenyl, 3-oxocyclohexenyl, 2,2-bis(ethoxycarbonyl)ethenyl, ethyl, n-propyl, n-butyl, 2-propyl, n-pentyl, 2-methylpropan-1-yl, 3,3-dimethylpropin-3-yl and 1,1-dimethylpropan-1-yl), (I) (where R₂ is fluoro, R₁, R₃ and R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is n-propyl), (I) (where R₁ is chloro, R₂-R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is ethyl, 3,3-dimethylpropin-3-yl or 1,1-dimethylpropan-1-yl), (I) (where R₁ is methyl, R₂-R₄ are hydrogen, A is a chemical bond, y and n are zero; and the moiety X-R₆ is ethyl), (I) (where R₁ is chloro, R₂ is methyl, R₃, R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is n-pentyl, 1,1-dimethylpropan-1-yl or 3,3-dimethylpropin-3-yl), (I) (where R₁-R₄ are hydrogen, A is CH₂, y and n are zero, and the moiety X-R₆ is ethyl, 3-propenyl (allyl), 3-hydroxylpropan-1-yl, 3-fluoropropan-1-yl or 3-(methylsulfonyloxy)propan-1-yl), (I) (where R₂ is bromo, R₁, R₃, R₄ are hydrogen, A is CH₂, y and n are zero, and the moiety X-R₆ is 3-propenyl), and (I) (where R₁ is chloro, R₂-R₄ are hydrogen, A is a chemical bond, y and n are zero, and the moiety X-R₆ is 3-amino-4-((2-chloropyridin-5-yl)oxy)butyl); and

(4) synergistic pesticidal mixtures, comprising (I), and a pesticide comprising organo(thio)phosphates, carbamates, pyrethroids, growth regulators, neonicotinoids, nicotinic receptor agonists/antagonists compounds, gamma amino butyric acid antagonist compounds, macrocyclic lactone insecticides, mitochondrial electron transport inhibitor I-III compounds, oxidative phosphorylation inhibitor compounds, molting disruptor compounds, mixed function oxidase inhibitor compounds, sodium channel blocker compounds, benclonthiaz, bifentazate, cartap, flonicamid, pyridalyl, pymetrozine, sulfur, thiocyclam, flubendiamide, cyenopyrafen, flupyrzafos, cyflumetofen, amidoflumet, hydrazone compounds of formula N-R₁aa-2, 2-dihalo-1-R₁bb-cyclo-propanecarboxamide-2-(2,6-dichloro- a, a, a-tri-fluoro-p-tolyl)hydrazone or N-R₁aa-2, 2-di(R₁cc)propionamide-2-(2,6-dichloro- a, a, a-trifluoro-p-tolyl)-hydrazone, or an anthranilamide compound of formula (III).

R₁aa, R₁cc = CH₃ or ethyl;

halo = chloro or bromo;

R₁bb = H or CH₃;

A1 = CH3, Cl, Br or I;
 X = C-H, C-Cl, C-F or N;
 Y1a = F, Cl or Br;
 Y1b = F, Cl or CF3;
 B1 = H, Cl, Br, I or CN;
 B2 = Cl, Br, CF3, OCH2CF3 or OCF2H; and
 R1B = H, CH3 or CH(CH3)2.

USE

USE - (I) are useful for: combating pests; protecting seed; and protecting growing plants from attack or infestation by pests, which are e.g. insects (claimed), arthropods, nematodes and arachnids. (I) are useful for protecting materials against infestation and/or destruction by the pests. The ability of (I) to combat pest was tested against *Aphis gossypii*. The result showed that 3-chloro-5-((S)-1-phenyl-azetidin-2-ylmethoxy)-pyridine showed over 90% mortality in comparison with untreated controls, at 300 ppm.

L62 ANSWER 19 OF 25 WPIX COPYRIGHT 2009 THOMSON REUTERS on STN
 ACCESSION NUMBER: 2008-C18580 [16] WPIX [Full-text](#)
 DOC. NO. CPI: C2008-062637 [16]
 TITLE: New quinoline derivatives, useful to treat, control, prevent or protect animals against infestation or infection by parasites, and to control e.g. insects, acarids or nematodes
 DERWENT CLASS: B02; B05; C02; C03
 INVENTOR: ANSPAUGH D D; CULBERTSON D L; GRAMMENOS W; KORADIN C; KUHN D G; LANGEWALD J; LOHMANN J K; OLOUMI-SADEGHI H; PARRA RAPADO L; PUHL M; RACK M; RHEINHEIMER J; VAN TUYL COTTER H; ANSPAUGH D; CULBERTSON D; KUHN D
 PATENT ASSIGNEE: (BADI-C) BASF AG; (BADI-C) BASF SE
 COUNTRY COUNT: 119

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2007104726	A1	20070920	(200816)*	EN	86[0]	
EP 2007727	A1	20081231	(200904)	EN		
TW 2008004286	A	20080116	(200908)	ZH		
KR 2008105159	A	20081203	(200915)	KO		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2007104726	A1	WO 2007-EP52262	20070312
EP 2007727	A1	EP 2007-726777	20070312
EP 2007727	A1	PCT Application	WO 2007-EP52262
TW 2008004286	A		20070314
KR 2008105159	A	PCT Application	WO 2007-EP52262
KR 2008105159	A		20081014

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 2007727	A1	Based on WO 2007104726 A
KR 2008105159	A	Based on WO 2007104726 A

PRIORITY APPLN. INFO: US 2006-782429P 20060315

INT. PATENT CLASSIF.:

IPC ORIGINAL:

A01N0043-34 [I,C]; A01N0043-34 [I,C]; A01N0043-42 [I,A];
 A61K0031-47 [I,A]; A61K0031-47 [I,C]; C07C0311-00 [I,C];
 C07C0311-15 [I,A]; C07D0215-00 [I,C]; C07D0215-00 [I,C];
 C07D0215-12 [I,A]; C07D0215-60 [I,A]; A01N0043-34 [I,C];
 A01N0043-42 [I,A]; C07D0215-00 [I,C]; C07D0215-12 [I,A];
 C07D0215-60 [I,A]

ECLA:

C07D0215-12; C07D0215-60

ICO:

M07D0215:12; M07D0215:60

BASIC ABSTRACT:

WO 2007/104726 A1 UPAB: 20090212

NOVELTY - Quinoline derivatives (I) and their N-oxides, enantiomers, diastereomers or their salts are new.

DETAILED DESCRIPTION - Quinoline derivatives of formula (I) and their N-oxides, enantiomers, diastereomers or their salts are new.

R1-R3 = halo, OH, CN, amino, nitro, 1-6C-alkyl, 2-6C-alkenyl, 2-6C-alkynyl, 3-7C-cycloalkyl, 3-7C-cycloalkyl-1-4C-alkyl, 1-6C-alkoxy, 2-6C-alkenyloxy, 2-6C-alkynyloxy, 1-4C-alkoxy-1-4C-alkoxy, 3-7C-cycloalkyl-1-4C-alkoxy, C(OH)(CF3)2, 1-6C-haloalkyl, 1-6C-haloalkoxy, 1-6C-alkylthio, 1-6C-haloalkylthio, 1-6C-alkylsulfanyl, 1-6C-haloalkylsulfanyl, 1-6C-alkylsulfonyl, 1-6C-haloalkylsulfonyl, C(R-a)=O, C(R-a)=NOR-b, C(=O)OR-x or C(=O)NR-xR-y;

R-a = H or 1-4C-alkyl;

R-b = H, 1-4C-alkyl, 2-4C-alkenyl, 2-4C-alkynyl, 1-4C-haloalkyl, or 2-4C-haloalkenyl;

R-x, R-y = H, 1-4C-alkyl, 1-4C-haloalkyl, 1-4C-alkoxy-1-4C-alkyl, 1-4C-thioalkyl-1-4C-alkyl, 1-4C-alkyl-S(=O)1-4C-alkyl, 1-4C-alkyl-S(=O)21-4C-alkyl, 3-6C-cycloalkyl, 1-4C-alkyl-3-6C-cycloalkyl, 3-6C-alkenyl, 3-6C-alkynyl;

R4-R7 = H, halo, CN, amino, nitro, OH, 1-6C-alkyl, 1-6C-alkoxy, 1-6C-haloalkyl, 1-6C-haloalkoxy, 1-6C-alkylthio, 1-6C-haloalkylthio, 1-6C-alkylsulfanyl, 1-6C-alkylsulfonyl, 1-6C-alkylsulfonyl, 1-6C-haloalkylsulfonyl, 1-6C-haloalkylsulfonyl or C(=O)OR-c;

R-c = H, 1-6C-alkyl, 2-6C-alkenyl or 2-6C-alkynyl;

m, n = 1-5; and

P = 0-5.

INDEPENDENT CLAIMS are included for:

- (1) the preparation of (I);
- (2) an intermediate quinoline amino sulfonyl phenyl compounds of formula (II);
- (3) a method for control of insects, acarid or nematodes by contacting the insect, acarid or nematode or their food supply, habitat, breeding ground or their locus, with (I);
- (4) a method of protecting growing plants from attack or infestation by insects, acarids or nematodes by applying (I) to the plants, or to the soil or water in which they are growing;
- (5) a method of protection of seed comprising contacting the seeds with (I);
- (6) seed comprising (I) 0.1 g to 10 kg per 100 kg of seeds; and
- (7) a method for treating, controlling, preventing or protecting animals against infestation or infection by parasites, comprising orally, topically or parenterally administering or applying (I) to the animals; and
- (8) synergistic pesticidal mixtures, comprising (I) and a pesticide e.g. organo(thio)phosphates, carbamates, pyrethroids, juvenile hormone mimics, nicotinic receptor agonists/antagonists compounds, gamma amino butyric acid gated chloride channel antagonist compounds, chloride channel activators, mitochondrial electron transport inhibitor (METI) I, II, and III compounds, uncouplers of oxidative phosphorylation, inhibitors of oxidative phosphorylation, moulting disruptors, synergists, sodium channel blocker compounds, fumigants, selective feeding blockers, mite growth inhibitors, chitin synthesis inhibitors, lipid biosynthesis inhibitors, octapaminergic

agonists, ryanodine receptor modulators, aluminum phosphide, amidoflumet, benclothiaz, benzoic acid, bifenazate, borax, bromopropylate, cyanide, cyenopyrafen, cyflumetofen, chinomethionate, dicofol, fluoroacetate, phosphine, pyridalyl, pyrifluquinazon, sulfur, tartar emetic; N-R-a-2,2-dihalo-1-R-bicyclo-propanecarboxamide-2-(2,6-dichloro- α,α,α -tri-fluoro-ptolyl) hydrazone or N-R-a-2,2-di(R-c)propionamide-2-(2,6-dichloro- α,α,α -tri-fluorop-tolyl)-hydrazone, (where R-a is methyl or ethyl, halo (chloro or bromo), R-b is hydrogen or methyl, and R-c is methyl or ethyl), chloranthraniliprole, 5-bromo-2-(3-chloro-pyridin-2-yl)-2H-pyrazole-3-carboxylic acid (4-cyano-2-methyl-6-methylcarbamo-phenyl)-amide and 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3,3,4,4,4-pentafluorobutyl)-malonodinitrile.

L2 = Cl, Br or I;

R4, R7 = H; and

R5, R6 = H, -CH3, F, Cl, -OCH3 or -OCF3.

ACTIVITY - Insecticide; Nematocide; Antiparasitic.

MECHANISM OF ACTION - None given.

USE - (I) are useful: for combating or controlling insects, acarids or nematodes; for protecting growing plants from attack or infestation by insects, acarids or nematodes; and for protecting seeds; for treating, controlling, preventing or protecting animals against infestation or infection by parasites (claimed). The ability of (I) for protecting animals against yellow fever mosquitoes (*Aedes aegypti*). The result showed that (2',4'-dichloro-biphenyl-4-sulfonic acid (quinolin-4-ylmethyl)-amide) exhibited 100% mortality at 1 ppm after 3 days.

ADVANTAGE - (I) exhibits synergistic effect in pesticidal mixtures.

(I) are effective pesticidal agents. MANUAL CODE: CPI: B04-A07C; B05-A01B; B05-A02; B05-B02A3; B05-B02C;

B05-C03; B05-C06; B06-D02; B06-F05; B07-D04C; B07-D08;
B10-A08; B10-A12C; B10-A15; B10-A18; B10-A19; B10-C02;
B10-C04E6; B10-E04B; B14-A02B9; B14-B02; B14-B03A;
B14-B04A; B14-B04B; B14-L01; B14-L06; B14-S09; C04-A07C;
C05-A01B; C05-A02; C05-B02A3; C05-B02C; C05-C03; C05-C06;
C06-D02; C06-F05; C07-D04C; C07-D08; C10-A08; C10-A12C;
C10-A15; C10-A18; C10-A19; C10-C02; C10-C04E6; C10-E04B;
C14-A02B9; C14-B02; C14-B03A; C14-B04A; C14-B04B;
C14-L01; C14-L06; C14-S09; C14-U02; N02-F02

IN ANSPAUGH D D; CULBERTSON D L; GRAMMENOS W; KORADIN C; KUHN D G; LANGEWALD J; LOHMANN J K; OLOUMI-SADEGHI H; PARRA RAPADO L; PUHL M; RACK M; RHEINHEIMER J; VAN TUYL COTTER H; ANSPAUGH D; CULBERTSON D; KUHN D
DETD DETAILED DESCRIPTION - Quinoline derivatives of formula (I) and their N-oxides, enantiomers, diastereomers or their salts are new.

R1-R3 = halo, OH, CN, amino, nitro, 1-6C-alkyl, 2-6C-alkenyl, 2-6C-alkynyl, 3-7C-cycloalkyl, 3-7C-cycloalkyl-1-4C-alkyl, 1-6C-alkoxy, 2-6C-alkenyloxy, 2-6C-alkynyloxy, 1-4C-alkoxy-1-4C-alkoxy, 3-7C-cycloalkyl-1-4C-alkoxy, C(OH)(CF3)2, 1-6C-haloalkyl, 1-6C-haloalkoxy, 1-6C-alkylthio, 1-6C-haloalkylthio, 1-6C-alkylsulfanyl, 1-6C-haloalkylsulfanyl, 1-6C-alkylsulfonyl, 1-6C-haloalkylsulfonyl, C(R-a)=O, C(R-a)=NOR-b, C(=O)OR-x or C(=O)NR-xR-y;

R-a = H or 1-4C-alkyl;

R-b = H, 1-4C-alkyl, 2-4C-alkenyl, 2-4C-alkynyl, 1-4C-haloalkyl, or 2-4C-haloalkenyl;

R-x, R-y = H, 1-4C-alkyl, 1-4C-haloalkyl, 1-4C-alkoxy-1-4C-alkyl, 1-4C-thioalkyl-1-4C-alkyl, 1-4C-alkyl-S(=O)1-4C-alkyl, 1-4C-alkyl-S(=O)21-4C-alkyl, 3-6C-cycloalkyl, 1-4C-alkyl-3-6C-cycloalkyl, 3-6C-alkenyl, 3-6C-alkynyl;

R4-R7 = H, halo, CN, amino, nitro, OH, 1-6C-alkyl, 1-6C-alkoxy, 1-6C-haloalkyl, 1-6C-haloalkoxy, 1-6C-alkylthio, 1-6C-haloalkylthio, 1-6C-alkylsulfanyl, 1-6C-haloalkylsulfanyl, 1-6C-alkylsulfonyl, 1-6C-haloalkylsulfonyl or C(=O)OR-c;

R-c = H, 1-6C-alkyl, 2-6C-alkenyl or 2-6C-alkinyl;

m, n = 1-5; and

P = 0-5.

INDEPENDENT CLAIMS are included for:

(1) the preparation of (I);

(2) an intermediate quinoline amino sulfonyl phenyl compounds of formula (II);

(3) a method for control of insects, acarid or nematodes by contacting the insect, acarid or nematode or their food supply, habitat, breeding ground or their locus, with (I);

(4) a method of protecting growing plants from attack or infestation by insects, acarids or nematodes by applying (I) to the plants, or to the soil or water in which they are growing;

(5) a method of protection of seed comprising contacting the seeds with (I);

(6) seed comprising (I) 0.1 g to 10 kg per 100 kg of seeds; and

(7) a method for treating, controlling, preventing or protecting animals against infestation or infection by parasites, comprising orally, topically or parenterally administering or applying (I) to the animals; and

(8) synergistic pesticidal mixtures, comprising (I) and a pesticide e.g. organo(thio)phosphates, car-bamates, pyrethroids, juvenile hormone mimics, nicotinic receptor agonists/antagonists compounds, gamma amino butyric acid gated chloride channel antagonist compounds, chloride channel activators, mitochondrial electron transport inhibitor (METI) I, II, and III compounds, uncouplers of oxidative phosphorylation, inhibitors of oxidative phosphorylation, moulting disruptors, synergists, sodium channel blocker compounds, fumigants, selective feeding blockers, mite growth inhibitors, chitin synthesis inhibitors, lipid biosynthesis inhibitors, octapaminergic agonists, ryanodine receptor modulators, aluminum phosphide, amidoflumet, benclonthiaz, benzoximate, bifentazate, borax, bromopropylate, cyanide, cyenopyrafen, cyflumetofen, chinomethionate, dicofol, fluoroacetate, phosphine, pyridalyl, pyrifluquinazon, sulfur, tartar emetic;
N-R-a-2,2-dihalo-1-R-bicyclo-propanecarboxamide-2-(2,6-dichloro-alpha,alpha,alpha-tri-fluoro-ptolyl) hydrazone or
N-R-a-2,2-di(R-c)propionamide-2-(2,6-dichloro-alpha,alpha,alpha-trifluorop-tolyl)-hydrazone, (where R-a is methyl or ethyl, halo (chloro or bromo), R-b is hydrogen or methyl, and R-c is methyl or ethyl),
chloranthraniliprole, 5-bromo-2-(3-chloro-pyridin-2-yl)-2H-pyrazole-3-carboxylic acid (4-cyano-2-methyl-6-methylcarbamoyl-phenyl)-amide and 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3,3,4,4,4-pentafluorobutyl)-malonodinitrile.

L2 = Cl, Br or I;

R4, R7 = H; and

R5, R6 = H, -CH3, F, Cl, -OCH3 or -OCF3.

L62	ANSWER 20 OF 25	WPIX COPYRIGHT 2009	THOMSON REUTERS on STN
ACCESSION NUMBER:	2008-H46453 [47]	WPIX	Full-text
DOC. NO. CPI:	C2008-234179 [47]		
DOC. NO. NON-CPI:	N2008-596091 [47]		
TITLE:	Pesticidal compositions, useful for combating pests, protecting growing plants from attack or infestation by pests and protecting seeds, comprises 3-pyridyl derivatives and a carrier		
DERWENT CLASS:	C02; S03		
INVENTOR:	ANSIPAUGH D D; BREUNINGER D; CULBERTSON D L; KUHN D G; OLOUMI-SADEGHI H; PARRA RAPADO L; POHLMAN M; PUHL M; RACK M; SCHMIDT T; VAN TU COTTER H; ANSPAUGH D; CULBERTSON D; KUHN D		

10/584354

PATENT ASSIGNEE: (BADI-C) BASF AG; (BADI-C) BASF SE
COUNTRY COUNT: 118

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2007085565	A1	20070802	(200847)*	EN	94[0]	
TW 2008000020	A	20080101	(200907)	ZH		
EP 1983830	A1	20081029	(200873)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2007085565	A1	WO 2007-EP50522	20070119
EP 1983830	A1	EP 2007-712059	20070119
EP 1983830	A1	PCT Application	WO 2007-EP50522 20070119
TW 2008000020	A	TW 2007-101807	20070117

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1983830	A1 Based on	WO 2007085565 A

PRIORITY APPLN. INFO:

US 2006-867637P	20061129
US 2006-762305P	20060126
US 2006-867287P	20061127
US 2006-762305P	20060126
US 2006-867287P	20061127
US 2006-867637P	20061129

INT. PATENT CLASSIF.:

IPC ORIGINAL: A01N0043-34 [I,C]; A01N0043-40 [I,A]; A01N0043-44 [I,A];
A01P0005-00 [I,A]; A01P0005-00 [I,C]; A01P0007-00 [I,A];
A01P0007-00 [I,C]; C07D0401-00 [I,C]; C07D0401-12 [I,A];
A01N0043-34 [I,C]; A01P0007-00 [I,C]; C07D0401-00 [I,C]

ECLA: A01N0043-40; A01N0043-44; C07D0401-12
ICO: M07D0401:12

BASIC ABSTRACT:

WO 2007085565 A1 UPAB: 20090205

NOVELTY - Pesticidal compositions (A) comprises 3-pyridyl derivatives (T) or their diastereomers, enantiomers or salts, and a carrier.

DETAILED DESCRIPTION - Pesticidal compositions (A) comprises 3-pyridyl derivatives (T) of formulae (I) and (II), or their diastereomers, enantiomers or salts, and a carrier.

X = O or S;

R1, R2 = H, halo, CN, NO2, 1-6C (halo)alkyl, 2-6C (halo)alkenyl, 2-6C (halo)alkynyl, 3-6C (halo)cycloalkyl, 3-6C (halo)cycloalkenyl, 1-6C-alkyl-3-6C-cycloalkyl, ORi, S(=O)Ri, S(=O)2Ri, NRiRj, C(=O)ORi, SiRjzRi3-z (where z is 0 to 3) or phenyl or 5-6-membered heteroaromatic ring optionally contain 1-4 heteroatoms of O, N or S or 3-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-3 groups of halo, amino, CN, Ri, ORi, S(=O)Ri or nitro;

Ri, Rj = H, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl 2-6C halo alkenyl, 2-6C alkynyl, 2-6C halo alkynyl, 3-6C cycloalkyl, 3-6C halo cycloalkyl, 3-6C cycloalkenyl, 3-6C halo cycloalkenyl, 1-6C haloalkoxy, 1-4C-alkoxy-1-6C-alkyl, 1-4C-alkylthio-1-6C-alkyl, 1-4C-alkylsulfanyl-1-6C-alkyl, 1-4C-alkylsulfonyl-1-6C-alkyl, 1-4C-haloalkoxy-1-6C-alkyl, 1-4C-haloalkylthio-1-6C-alkyl, (1-4C-

alkoxy)carbonyl-1-6C-alkyl, (di)(1-4C-alkyl)amino-1-6C-alkyl, 3-6C-cycloalkyl-1-6C-alkyl, phenyl-1-6C-alkyl, or 1-6C alkyl (all optionally substituted with 1-3 CN groups);

R3 = H, halo or 1-6C alkyl;

R4 = H or 1-6C alkyl;

R5, R6 = H, halo, CN or 1-6C alkyl;

R7 = 1-6C alkyl, 2-6C alkenyl, 2-6C alkynyl, 3-6C cycloalkyl, 3-6C cycloalkenyl, 1-6C haloalkyl, 2-6C haloalkenyl, 2-6C haloalkynyl, 3-6C halocycloalkyl, 3-6C halocycloalkenyl or -C(=G)Ra, -C(=G)ORa, -C(=G)NRaRb, -C(=NORa)Rb, 3-6C-cycloalkyl-1-6C-alkyl or phenyl or 3-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, S or N or 5-6-membered heteroaromatic ring system optionally contain 1-4 heteroatoms of O, N or S, phenyl, heterocyclic ring or heteroaromatic ring may be bonded via 1-4C alkyl, where phenyl or heteroaromatic ring or the heterocyclic ring may be fused to a ring of phenyl or 5-6-membered or aromatic heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S, (where R7 are unsubstituted or the H atoms in these groups optionally be replaced with any combination of groups Rc);

G = O or S;

Ra, Rb = halo, CN, NO2, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 3-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl, ORk, SRk, S(=O)Rk, S(=O)2Rk, S(=O)2NRkRm, C(=O)Rk, C(=O)ORk, C(=O)NRkRm, C(=NORk)Rm, -C(=G)NRk-NRmRn, SiRkzRm3-z or phenyl or 5-6-membered heteroaromatic ring (optionally contain 1-4 heteroatoms of O, N or S) or 4-7-membered heterocyclic ring (optionally contain 1-3 heteroatoms of O, N or S), where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-5 halo;

z = 0-3;

Rk, Rm, Rn = H, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 3-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl;

Rc = halo, CN, NO2, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 3-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl, ORk, SRk, S(=O)Rk, S(=O)2Rk, NRkRm, N(ORk)Rm, -S(=O)2NRkRm, C(=O)Ra, C(=O)ORk, C(=O)NRkRm, C(=NORk)Rm, -NRkC(=G)Rm, -N(ORk)C(=G)Rm, -N(C(=G)Rk)C(=G)Rm, -NRkC(=G)ORm, -N(ORk)C(=G)ORm, -C(=G)NRk-NRmRn, -NRkSO2Rm, SiRkzRm3-z or phenyl or 5-6-membered heteroaromatic ring optionally contain 1-4 heteroatoms of O, N or S, 4-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S, where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-5 halo; and

x, y1 = 0 or 1.

INDEPENDENT CLAIMS are included for:

(1) a method for controlling pests comprising contacting the pests or their food supply, habitat, breeding ground or their locus with (A);

(2) a method for protecting growing plants from attack or infestation by pests comprising applying (A) to the plant, or to the soil or the water in which the plant is growing;

(3) a method of protection of seed comprising contacting the seeds with (A);

(4) a seed comprising (T) at 0.1 g-10 kg/100 kg of seeds;

(5) the preparation of (T) (where y is 0) comprising reacting amine compound of formula (II-1) with an activated carboxylic acid derivative (R7C(=O)Y1) in the presence of a base to give a pyridyl derivative of formula (I-1); and

(6) a synergistic pesticidal mixtures comprising (T) and pesticide such as organo(thio)phosphates, carbamates, pyrethroids, growth regulators, neonicotinoids, nicotinic receptor agonists/antagonists compounds, gamma-aminobutyric acid antagonist compounds, macrocyclic lactone insecticides,

mitochondrial electron transport inhibitor (METI) I compounds such as fenazaquin, pyridaben, tebufenpyrad, tolfenpyrad and flufenimer, METI II and III compounds such as acequinoacyl, fluacyprim and hydramethylnon, oxidative phosphorylation inhibitor compounds, moulting disruptor compounds, mixed function oxidase inhibitor compounds, sodium channel blocker compounds, benclothiaz, bifentazate, cartap, flonicamid, pyridalyl, pymetrozine, sulfur, thiocyclam, flubendiamide, cyenopyrafen, flupyrzafos, cyflumetofen, amidoflumet, amine compound of formula (N-Ra-2,2-dihalo-1-Rb cyclopropanecarboxamide-2-(2,6-dichloro- alpha , alpha , alpha -tri-fluoro-p-tolyl)hydrazone), (N-Ra-2,2-di(Rc)propionamide-2-(2,6-dichloro- alpha , alpha , alpha -trifluoro-p-tolyl)-hydrazone) and anthranilamide compounds of formula (III).

Y1 = OH, leaving group such as Cl or Br, Ord, OC(=O)Re or imidazole;

Rd = 1-6C alkyl or N-hydroxybenzotriazole;

Re = 1-6C alkyl or phenyl;

Ra = methyl, ethyl or halo (Cl or Br);

Rb = H or methyl; and

Rc = methyl or ethyl;

Al = CH₃, Cl, Br or I;

X = C-H, C-Cl, C-F or N;

Y1a = F, Cl or Br;

Y1b = F, Cl or CF₃;

B1 = H, Cl, Br, I or CN;

B2 = Cl, Br, CF₃, OCH₂CF₃ or OCF₂H; and

RB1 = H, CH₃ or CH(CH₃)₂.

ACTIVITY - Antidote.

MECHANISM OF ACTION - None given.

USE - (A) is useful for combating/controlling pests (preferably insects), protecting growing plants from attack or infestation by pests and for protecting seeds (claimed). The ability of (I) to control pest was tested against cowpea aphid in cowpea plants. The results showed that (2-(5-fluoro-pyridin-3-yloxy)methyl)-azetidin-1-yl)-(tetrahydro-furan-3-yl)-methanone exhibited 90% mortality.

ADVANTAGE - (A) have synergistic effect. (A) are effective for controlling pests through both contact and ingestion. MANUAL CODE: CPI: C05-C06; C06-D06; C07-H; C10-A08; C10-A10; C10-A12A;

C10-G02; C11-C01D; C14-B04B; C14-M01E; C14-S09; C14-S18

EPI: S03-E14M

IN ANSPAUGH D D; BREUNINGER D; CULBERTSON D L; KUHN D G; OLOUMI-SADEGHI H; PARRA RAPADO L; POHLMAN M; PUHL M; RACK M; SCHMIDT T; VAN TU COTTER H; ANSPAUGH D; CULBERTSON D; KUHN D

DETD DETAILED DESCRIPTION - Pesticidal compositions (A) comprises 3-pyridyl derivatives (I) of formulae (I) and (II), or their diastereomers, enantiomers or salts, and a carrier.

X = O or S;

R1, R2 = H, halo, CN, NO₂, 1-6C (halo)alkyl, 2-6C (halo)alkenyl, 2-6C (halo)alkynyl, 3-6C (halo)cycloalkyl, 3-6C (halo)cycloalkenyl, 1-6C-alkyl-3-6C-cycloalkyl, ORi, SRi, S(=O)Ri, S(=O)₂Ri, NRiRj, C(=O)ORi, SiRjzRi3-z (where z is 0 to 3) or phenyl or 5-6-membered heteroaromatic ring optionally contain 1-4 heteroatoms of O, N or S or 3-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-3 groups of halo, amino, CN, R1, ORi, SRi or nitro;

Ri, Rj = H, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl 2-6C halo alkenyl, 2-6C alkynyl, 2-6C halo alkynyl, 3-6C cycloalkyl, 3-6C halo cycloalkyl, 3-6C cycloalkenyl, 3-6C halo cycloalkenyl, 1-6C haloalkoxy, 1-4C-alkoxy-1-6C-alkyl, 1-4C-alkylthio-1-6C-alkyl, 1-4C-alkylsulfinyl-1-6C-alkyl, 1-4C-alkylsulfonyl-1-6C-alkyl, 1-4C-haloalkoxy-1-6C-alkyl, 1-4C-haloalkylthio-1-6C-alkyl,

(1-4C-alkoxy)carbonyl-1-6C-alkyl, (di)(1-4C-alkyl)amino-1-6C-alkyl, 3-6C-cycloalkyl-1-6C-alkyl, phenyl-1-6C-alkyl, or 1-6C alkyl (all optionally substituted with 1-3 CN groups);

R3 = H, halo or 1-6C alkyl;

R4 = H or 1-6C alkyl;

R5, R6 = H, halo, CN or 1-6C alkyl;

R7 = 1-6C alkyl, 2-6C alkenyl, 2-6C alkynyl, 3-6C cycloalkyl, 3-6C cycloalkenyl, 1-6C haloalkyl, 2-6C haloalkenyl, 2-6C haloalkynyl, 3-6C halocycloalkyl, 3-6C halocycloalkenyl or -C(=G)Ra, -C(=G)ORa, -C(=G)NRaRb, -C(=NORa)Rb, 3-6C-cycloalkyl-1-6C-alkyl or phenyl or 3-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, S or N or 5-6-membered heteroaromatic ring system optionally contain 1-4 heteroatoms of O, N or S, phenyl, heterocyclic ring or heteroaromatic ring may be bonded via 1-4C alkyl, where phenyl or heteroaromatic ring or the heterocyclic ring may be fused to a ring of phenyl or 5-6-membered or aromatic heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S, (where R7 are unsubstituted or the H atoms in these groups optionally be replaced with any combination of groups Rc);

G = O or S;

Ra, Rb = halo, CN, NO2, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 2-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl, ORk, SRk, S(=O)Rk, S(=O)2Rk, S(=O)2NRkRm, C(=O)Rk, C(=O)ORk, C(=O)NRkRm, C(=NORk)Rm, -C(=G)NRk-NRmRn, SiRkzRm3-z or phenyl or 5-6-membered heteroaromatic ring (optionally contain 1-4 heteroatoms of O, N or S) or 4-7-membered heterocyclic ring (optionally contain 1-3 heteroatoms of O, N or S), where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-5 halo;

z = 0-3;

Rk, Rm, Rn = H, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 2-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl;

Rc = halo, CN, NO2, 1-6C alkyl, 1-6C haloalkyl, 2-6C alkenyl, 2-6C haloalkenyl, 2-6C alkynyl, 2-6C haloalkynyl, 3-6C cycloalkyl, 3-6C halocycloalkyl, 3-6C cycloalkenyl, 3-6C halocycloalkenyl, ORk, SRk, S(=O)Rk, S(=O)2Rk, NRkRm, N(ORk)Rm, -S(=O)2NRkRm, C(=O)Rk, C(=O)ORk, C(=O)NRkRm, C(=NORk)Rm, -NRkC(=G)Rm, -N(ORk)C(=G)Rm, -N(C(=G)Rk)C(=G)Rm, -NRkC(=G)ORm, -N(ORk)C(=G)ORm, -C(=G)NRk-NRmRn, -NRkSO2Rm, SiRkzRm3-z or phenyl or 5-6-membered heteroaromatic ring optionally contain 1-4 heteroatoms of O, N or S, 4-7-membered heterocyclic ring optionally contain 1-3 heteroatoms of O, N or S, where the carbon atoms in phenyl or in the heteroaromatic or heterocyclic ring may be substituted with 1-5 halo; and

x, y1 = 0 or 1.

INDEPENDENT CLAIMS are included for:

(1) a method for controlling pests comprising contacting the pests or their food supply, habitat, breeding ground or their locus with (A);

(2) a method for protecting growing plants from attack or infestation by pests comprising applying (A) to the plant, or to the soil or the water in which the plant is growing;

(3) a method of protection of seed comprising contacting the seeds with (A);

(4) a seed comprising (T) at 0.1 g-10 kg/100 kg of seeds;

(5) the preparation of (T) (where y is 0) comprising reacting amine compound of formula (II-1) with an activated carboxylic acid derivative (R7C(=O)Y1) in the presence of a base to give a pyridyl derivative of formula (I-1); and

(6) a synergistic pesticidal mixtures comprising (T) and pesticide such as organo(thio)phosphates, carbamates, pyrethroids, growth regulators, neonicotinoids, nicotinic receptor agonists/antagonists

compounds, gamma-aminobutyric acid antagonist compounds, macrocyclic lactone insecticides, mitochondrial electron transport inhibitor (METI) I compounds such as fenazaquin, pyridaben, tebufenpyrad, tolfenpyrad and flufenimer, METI II and III compounds such as acequinocyl, fluacyprim and hydramethylnon, oxidative phosphorylation inhibitor compounds, moulting disruptor compounds, mixed function oxidase inhibitor compounds, sodium channel blocker compounds, benclothiaz, bifentazate, cartap, flonicamid, pyridalyl, pymetrozine, sulfur, thiocyclam, flubendiamide, cyenopyrafen, flupyrzafos, cyflumetofen, amidoflumet, amine compound of formula (N-Ra-2,2-dihalo-1-Rb cyclo-propanecarboxamide-2-(2,6-dichloro- alpha , alpha , alpha -tri-fluoro-p-tolyl)hydrazone), (N-Ra-2,2-di(Rc)propionamide-2-(2,6-dichloro- alpha , alpha , alpha -trifluoro-p-tolyl)-hydrazone) and anthranilamide compounds of formula (III).

Y1 = OH, leaving group such as Cl or Br, ORd, OC(=O)Re or imidazole;
 Rd = 1-6C alkyl or N-hydroxybenzotriazole;
 Re = 1-6C alkyl or phenyl;
 Ra = methyl, ethyl or halo (Cl or Br);
 Rb = H or methyl; and
 Rc = methyl or ethyl;
 A1 = CH3, Cl, Br or I;
 X = C-H, C-Cl, C-F or N;
 Y1a = F, Cl or Br;
 Y1b = F, Cl or CF3;
 B1 = H, Cl, Br, I or CN;
 B2 = Cl, Br, CF3, OCH2CF3 or OCF2H; and
 RB1 = H, CH3 or CH(CH3)2.

USE

USE - (A) is useful for combating/controlling pests (preferably insects), protecting growing plants from attack or infestation by pests and for protecting seeds (claimed). The ability of (I) to control pest was tested against cowpea aphid in cowpea plants. The results showed that (2-(5-fluoro-pyridin-3-ylloxymethyl)-azetidin-1-yl)-(tetrahydro-furan-3-yl)-methanone exhibited 90% mortality.

L62 ANSWER 21 OF 25 WPIX COPYRIGHT 2009 THOMSON REUTERS on STN
 ACCESSION NUMBER: 2007-499228 [49] WPIX [Full-text](#)
 CROSS REFERENCE: 2007-777100
 DOC. NO. CPI: C2007-183619 [49]
 TITLE: Preparation of fluorinated m-nitro-benzoic acid chloride compound, useful to prepare sulfonamide compound, comprises reacting a fluorinated m-nitro-benzoic acid compound with a chlorinating agent in the presence of a phosphine derivative
 E11; E14; J04
 DERWENT CLASS: GEBHARDT J; KEIL M; LOEHR S; MAYER G; RACK M;
 INVENTOR: SCHMIDT T; WEVERS J H
 PATENT ASSIGNEE: (BADI-C) BASF AG
 COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
DE 102005057681	A1	20070606	(200749)*	DE	20	[0]

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

PRIORITY APPLN. INFO: DE 2005-102005057681 20051201

INT. PATENT CLASSIF.:

IPC ORIGINAL: B01J0031-06 [I,A]; B01J0031-06 [I,C]; C07C0201-00 [I,C];
C07C0201-12 [I,A]; C07C0205-00 [I,C]; C07C0205-58 [I,A]
ECLA: C07C0205-58; C07C0323-34
ICO: M07C0307:06

BASIC ABSTRACT:

DE 102005057681 A1 UPAB: 20070801

NOVELTY - Preparation of fluorinated m-nitro-benzoic acid chloride compound (I) comprises reacting a fluorinated m-nitro-benzoic acid compound (II) with a chlorinating agent, in the presence of a catalytic amount of phosphine derivative (III).

DETAILED DESCRIPTION - Preparation of fluorinated m-nitro-benzoic acid chloride compound of formula (I) comprises reacting a fluorinated m-nitro-benzoic acid compound of formula (II) with a chlorinating agent, in the presence of a catalytic amount of phosphine derivative (III) of formula (Ra-P(=Xn)(Rb)-Rc).

R1-R4 = H, halo, CN, NO2, 1-6C alkyl, 1-6C haloalkyl, 1-6C alkoxy or 1-6C haloalkoxy (where at least one of the residue is F);

Ra-Rc = 1-6C alkyl or phenyl (optionally substituted by 1-4C alkyl);

X = O or two single bonded Cl atom; and

n = 0 or 1.

An INDEPENDENT CLAIM is included for the preparation of a sulfonamide compound of formula (V) comprising reacting (I) with an aminosulfone compound of formula (NH2-SO2NR5R6) (VI).

R5, R6 = H, 1-6C alkyl (preferred), 3-6C alkenyl, 3-6C alkynyl, 3-7C cycloalkyl, 3-7C cycloalkenyl, 1-6C alkoxy, phenyl or benzyl.

USE - (I) is useful in the preparation of sulfonamide compound (claimed).

ADVANTAGE - The catalyst used in the process increases the yield of (I) and decreases the reaction temperature. The process reduces the splitting of fluoride and provides (I) with high purity. MANUAL CODE: CPI: E10-A08A; E10-A08C; E10-A25B1; E11-F; J04-E01;

N05-E01; N07-D09

IN GEBHARDT J; KEIL M; LOEHR S; MAYER G; RACK M; SCHMIDT T; WEVERS J H

L62 ANSWER 22 OF 25 WPXI COPYRIGHT 2009 THOMSON REUTERS ON STN

ACCESSION NUMBER: 2006-065874 [07] WPXI [Full-text](#)

DOC. NO. CPI: C2006-024116 [07]

TITLE: Preparation of 4-trifluoromethyl-2(1H)-pyridinone useful to synthesize intermediate of herbicide involves contacting 1,1,1-trifluorobut-3-en-2-one or 1,1,1-trifluorobutan-2-one derivative with trialkyl phosphonoacetate followed by cyclizing

C02

DERWENT CLASS: GONZALEZ M A; GORMAN D B; GULLO M F; HAMILTON C T; ROTH G A; GEBHARDT J; GOETZ N; JAEDICKE H; MAYER G; RACK M

PATENT ASSIGNEE: (GONZ-I) GONZALEZ M A; (GORM-I) GORMAN D B; (GULL-I) GULLO M F; (HAMI-I) HAMILTON C T; (ROTH-I) ROTH G A; (DOWC-C) DOW AGROSCIENCES LLC

COUNTRY COUNT: 109

PATENT INFORMATION:

PATENT NO	KIND DATE	WEEK	LA	PG	MAIN IPC
US 20050288511	A1 20051229 (200607)*	EN	9	10	
WO 2006012320	A1 20060202 (200614)	EN			

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 20050288511 A1	Provisional	US 2004-583002P	20040625
US 20050288511 A1		US 2005-166485	20050624
WO 2006012320 A1		WO 2005-US22539	20050624
US 7488828 B2		US 2005-166485	20050624

PRIORITY APPLN. INFO: US 2005-166485 20050624
US 2004-583002P 20040625

INT. PATENT CLASSIF.:
IPC ORIGINAL: C07D0213-00 [I,C]; C07D0213-64 [I,A]; C07D0211-00 [I,C];
C07D0211-72 [I,A]
IPC RECLASSIF.: C07D0213-00 [I,C]; C07D0213-08 [I,A]
ECLA: C07D0213-64A
USCLASS NCLM: 546/250.000
BASIC ABSTRACT:

US 20050288511 A1 UPAB: 20090307

NOVELTY - Preparation of 4-trifluoromethyl-2(1H)-pyridinone involves contacting either 4-alkoxy-1,1,1-trifluorobut-3-en-2-one or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one, with trialkyl phosphonoacetate in the presence of a base and an alcohol or glycol solvent; and cyclizing the resultant mixture of condensation products.

DETAILED DESCRIPTION - Preparation of 4-trifluoromethyl-2(1H)-pyridinone (I) involves:

(1) contacting either a 4-alkoxy-1,1,1-trifluorobut-3-en-2-one of formula CF₃-C(=O)-CH=CH-OR (ia) or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one of CF₃-C(=O)-CH₂-CH(OR)₂ (ib), with a trialkyl phosphonoacetate of (RO)₂P(=O)-CH₂-C(=O)OR (ic) in the presence of a base and an alcohol or glycol solvent to form a mixture of condensation products of formulae CF₃-C(CH₂-CO₂R)=CH-CH(OR)₂ (iia), and E and Z isomers of CF₃-C(=CH-CO₂R)-CH₂-CH(OR)₂ (iib); and cyclizing the mixture of condensation products.

R=1-4C alkyl.

USE - For preparation of 4-trifluoromethyl-2(1H)-pyridinone (claimed), which is useful for synthesis of intermediates such as 2-methoxy-4-trifluoromethylpyridine required for preparation of herbicides.

ADVANTAGE - The method enables efficient synthesis of 4-trifluoromethyl-2(1H)-pyridinone at high yield from non-pyridine source; and can be conveniently performed without any additional solvents at reflux temperature.

MANUAL CODE: CFI: C07-D04B; C07-D04D

IN GONZALEZ M A; GORMAN D B; GULLO M F; HAMILTON C T; ROTH G A; GEBHARDT J; GOETZ N; JAEDICKE H; MAYER G; RACK M

NOV NOVELTY - Preparation of 4-trifluoromethyl-2(1H)-pyridinone involves contacting either 4-alkoxy-1,1,1-trifluorobut-3-en-2-one or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one, with trialkyl phosphonoacetate in the presence of a base and an alcohol or glycol solvent; and cyclizing the resultant mixture of condensation products.

DETD DETAILED DESCRIPTION - Preparation of 4-trifluoromethyl-2(1H)-pyridinone (I) involves:

(1) contacting either a 4-alkoxy-1,1,1-trifluorobut-3-en-2-one of formula CF₃-C(=O)-CH=CH-OR (ia) or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one of CF₃-C(=O)-CH₂-CH(OR)₂ (ib), with a trialkyl phosphonoacetate of (RO)₂P(=O)-CH₂-C(=O)OR (ic) in the presence of a base and an alcohol or glycol solvent to form a mixture of condensation products of formulae CF₃-C(CH₂-CO₂R)=CH-CH(OR)₂ (iia), and E and Z isomers of CF₃-C(=CH-CO₂R)-CH₂-CH(OR)₂ (iib); and cyclizing the mixture of condensation products.

10/584354

R=1-4C alkyl.

USE

USE - For preparation of 4-trifluoromethyl-2(1H)-pyridinone (claimed), which is useful for synthesis of intermediates such as 2-methoxy-4-trifluoromethylpyridine required for preparation of herbicides.

ADV

ADVANTAGE - The method enables efficient synthesis of 4-trifluoromethyl-2(1H)-pyridinone at high yield from non-pyridine source; and can be conveniently performed without any additional solvents at reflux temperature.

Member(0001)

ABEN

UPAA 20060130

4-Trifluoromethyl-2(1H)-pyridinone is prepared by reaction of 4-alkoxy-1,1,1-trifluorobut-3-en-2-one or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one with a trialkyl phosphonoacetate followed by cyclization.

Member(0002)

ABEN

UPAA 20060227

4-Trifluoromethyl-2(1H)-pyridinone is prepared by reaction of 4-alkoxy-1,1,1-trifluorobut-3-en-2-one or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one with a trialkyl phosphonoacetate followed by cyclization.

Member(0002)

ABFR

UPAA 20060227

Une 4-trifluoromethyl-2(1 H)-pyridinone est preparee par reaction de 4-alcoxy-1,1,1-trifluorobut-3-en-2-one ou d'une 4,4-dialcoxy-1,1,1-trifluorobutan-2-one avec un trialkyle phosphonoacetate suivie d'une cyclisation.

Member(0003)

ABEN

UPAA 20090307

4-Trifluoromethyl-2(1H)-pyridinone is prepared by reaction of 4-alkoxy-1,1,1-trifluorobut-3-en-2-one or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one with a trialkyl phosphonoacetate followed by cyclization.

L62 ANSWER 23 OF 25

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ACCESSION NUMBER:

2000-411669 [35] WPIX Full-text

CROSS REFERENCE:

1999-592080; 2000-053067

DOC. NO. CPI:

C2000-124654 [35]

TITLE:

High yield preparation of isoxazolin-3-yl-acyl benzenes useful as plant protectants, e.g. herbicides, by multi-stage process via several new intermediates

DERWENT CLASS:

C02; C03

INVENTOR:

BAUMANN E; GEBHARDT J; GOETZ N; GOTZ N; HAGEN H; KEIL M; LOCHTMAN R; MIBLITZ U; MISSLITZ U; RACK M; VON DEYN W; WITSCHEL M

PATENT ASSIGNEE:

(BADI-C) BASF AG; (BAUM-I) BAUMANN E; (GEBH-I) GEBHARDT J; (GOTZ-I) GOTZ N; (HAGE-I) HAGEN H; (KEIL-I) KEIL M; (LOCH-I) LOCHTMAN R; (MIBL-I) MIBLITZ U; (MISS-I) MISSLITZ U; (RACK-I) RACK M; (VDEY-I) VON DEYN W; (WITS-I) WITSCHEL M

COUNTRY COUNT:

88

PATENT INFORMATION:

PATENT NO

KIND DATE

WEEK

LA PG

MAIN IPC

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WO 2000029394 A1 20000525 (200035)* DE 68[0]
AU 2000016515 A 20000605 (200042) EN
EP 1129082 A1 20010905 (200151) DE
US 6469176 B1 20021022 (200273) EN
JP 2002529540 W 20020910 (200274) JA 71
US 20030028033 A1 20030206 (200318)# EN
US 20030220505 A1 20031127 (200378) EN
US 6706886 B2 20040316 (200420) EN
EP 1129082 B1 20040929 (200464) DE
DE 59910677 G 20041104 (200474) DE

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APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2000029394 A1		WO 1999-EP8746	19991112
DE 59910677 G		DE 1999-59910677	19991112
EP 1129082 A1		EP 1999-959276	19991112
EP 1129082 B1		EP 1999-959276	19991112
DE 59910677 G		EP 1999-959276	19991112
US 6706886 B2 Div Ex		US 1999-831400	19991112
EP 1129082 A1		WO 1999-EP8746	19991112
US 6469176 B1		WO 1999-EP8746	19991112
JP 2002529540 W		WO 1999-EP8746	19991112
US 20030220505 A1 Div Ex		WO 1999-EP8746	19991112
US 6706886 B2 Div Ex		WO 1999-EP8746	19991112
EP 1129082 B1		WO 1999-EP8746	19991112
DE 59910677 G		WO 1999-EP8746	19991112
AU 2000016515 A		AU 2000-16515	19991112
JP 2002529540 W		JP 2000-582381	19991112
US 6469176 B1		US 2001-831400	20010509
US 20030220505 A1 Div Ex		US 2001-831400	20010509
US 20030028033 A1 Div Ex		US 2001-831400	20010509
US 20030220505 A1 Div Ex		US 2002-223019	20020819
US 6706886 B2 Div Ex		US 2002-223019	20020819
US 20030028033 A1		US 2002-223019	20020819
US 20030220505 A1		US 2003-436739	20030514
US 6706886 B2		US 2003-436739	20030514

FILING DETAILS:

PATENT NO	KIND	PATENT NO
DE 59910677 G	Based on	EP 1129082 A
US 20030220505 A1	Div ex	US 6469176 B
US 6706886 B2	Div ex	US 6469176 B
US 20030028033 A1	Div ex	US 6469176 B
AU 2000016515 A	Based on	WO 2000029394 A
EP 1129082 A1	Based on	WO 2000029394 A
US 6469176 B1	Based on	WO 2000029394 A
JP 2002529540 W	Based on	WO 2000029394 A
EP 1129082 B1	Based on	WO 2000029394 A
DE 59910677 G	Based on	WO 2000029394 A

PRIORITY APPLN. INFO: WO 1999-EP3006 19990504
 DE 1998-19852095 19981112
 US 2002-223019 20020819

INT. PATENT CLASSIF.:
 MAIN: C07D261-04; C07D413-10

IPC RECLASSIF.: C07B0061-00 [I,A]; C07B0061-00 [I,C]; C07C0251-00 [I,C];
 C07C0251-40 [I,A]; C07C0251-48 [I,A]; C07C0319-00 [I,C];
 C07C0319-14 [I,A]; C07C0323-00 [N,C]; C07C0323-09 [N,A];
 C07D0261-00 [I,C]; C07D0261-00 [I,C]; C07D0261-04 [I,A];
 C07D0261-04 [I,A]; C07D0261-08 [I,A]; C07D0413-00 [I,C];
 C07D0413-00 [I,C]; C07D0413-10 [I,A]; C07D0413-10 [I,A]
 ECLA: C07C0251-48; C07C0319-14; C07D0261-04; C07D0261-08;
 C07D0413-10+261+231
 ICO: M07C0323:09; M07D0261:04; M07D0261:08; M07D0413:10
 USCLASS NCLM: 548/240.000
 NCLS: 548/364.100
 JAP. PATENT CLASSIF.:
 MAIN/SEC.: C07B0061-00 300; C07D0261-04; C07D0413-10
 FTERM CLASSIF.: C04056; 4C063; 4H039; 4C056/AA01; 4C063/AA01; 4C056/AB01;
 4C056/AC01; 4C056/AD01; 4C056/AE02; 4C056/AF01;
 4C063/BB06; 4H039/CA71; 4H039/CB30; 4C063/CC51;
 4C063/DD22; 4C063/EE03; 4C063/EE05

BASIC ABSTRACT:

WO 2000029394 A1 UPAB: 20050705

NOVELTY - A multi-stage process for preparing 3-(isoxazolin-3-yl)-4-thio-(heterocyclic acyl)-benzenes (I) comprises preparing intermediates of formula (VI) followed by halogenating, thioalkylating, oxidizing and acylating.

DETAILED DESCRIPTION - The preparation of 3-(isoxazolin-3-yl)-4-thio-(heterocyclic acyl)-benzenes of formula (I) involves preparing 2-(isoxazolin-3-yl)-aniline intermediates of formula (VI) followed by halogenating, thioalkylating, oxidizing and acylating.

n = 0-2;

R1-R5 = H or 1-6C alkyl; or

R4 + R5 = bond;

R6 = heterocycle.

INDEPENDENT CLAIMS are included for:

(1) new intermediates of formulae (III), (XII), (X) and (XV);

(2) the preparation of benzaldoxime derivatives of formula (XV') by reacting a toluene derivative of formula (XVI) with an organic nitrite R-O-NO in presence of base, where the oxime group of (XV') is optionally subsequently converted into the corresponding aldehyde, nitrile or nitrile oxide group;

(3) the preparation of thioethers of formula (XIX) by reacting anilines of formula (XX) with dialkyl disulfides of formula R'2SSR'2 (VII) in presence of a catalyst (specifically copper powder or elemental copper).

A = amino, NO2 or SR2;

R'1, R'2 = 1-6C alkyl;

R'1 = H, 1-6C alkyl, halo, 1-6C alkoxy or 1-6C alkylthio;

X = NO2 or S(O)nRy;

X' = S(O)nRy;

Rx, Ry = inert groups;

R'x = H, Cl or Br in the para-position;

n' = 2;

m = 0-4;

m' = 1;

m'' = 0-5; and

R = aliphatic or aromatic.

ACTIVITY - Herbicidal.

MECHANISM OF ACTION - None given.

USE - (I) are plant protectants, e.g. herbicides as described in WO9831681. (XV) are intermediates for (I) and related compounds; and (XIX) are intermediates for (I), other plant protectants and pharmaceuticals.

ADVANTAGE - Compared with the method of WO9831681, the present preparation has fewer stages and gives a higher overall yield. The starting materials are readily available. All the stages give high yield and are suitable

for industrial use. An inexpensive, economical and safe method for the large-scale preparation of (I) is provided. MANUAL CODE: CPI: C07-E01; C07-H; C10-A18; C10-H01; C14-V01

IN BAUMANN E; GEBHARDT J; GOETZ N; GOTZ N; HAGEN H; KEIL M; LOCHTMAN R; MIBLITZ U; MISSLITZ U; RACK M; VON DEYN W; WITSCHEL M

L62 ANSWER 24 OF 25 WPIX COPYRIGHT 2009 THOMSON REUTERS ON STN

ACCESSION NUMBER: 1999-592080 [51] WPIX Full-text

CROSS REFERENCE: 2000-053067; 2000-411669

DOC. NO. CPI: C1999-173153 [51]

TITLE: Preparation of benzoyl pyrazole derivative herbicides, in single stage from hydroxypyrazole, bromobenzene and carbon monoxide

DERWENT CLASS: C02

INVENTOR: GEBHARDT J; RHEINHEIMER J; VON DEYN W; GOTZ N; HAGEN H; KEIL M; LOCHTMAN R; RACK M; WITSCHEL M

PATENT ASSIGNEE: (BADI-C) BASF AG

COUNTRY COUNT: 2

PATENT INFORMATION:

PATENT NO	KIND DATE	WEEK	LA	PG	MAIN IPC
DE 19820722	C1 19991104 (199951)*	DE	6	0	
IN 2000CN00738	P4 20070511 (200747)	EN			

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 19820722	C1	DE 1998-19820722	19980511
IN 2000CN00738	P4	WO 1999-EP3006	19990504
IN 2000CN00738	P4	IN 2000-CN738	20001128

PRIORITY APPLN. INFO: DE 1998-19820722 19980511

INT. PATENT CLASSIF.:

MAIN: C07D261-04

IPC RECLASSIF.: C07C [I,S]; C07D [I,S]; C07D0413-00 [I,C]; C07D0413-10 [I,A]

BASIC ABSTRACT:

DE 19820722 C1 UPAB: 20050523

NOVELTY - Preparation of 4-(4-alkylsulfonyl-3-isoxazolyl- benzoyl)-5-hydroxypyrazole derivatives (I) involves reacting a hydroxypyrazole (II) with a bromobenzene (III) in presence of carbon monoxide, a palladium catalyst, a potassium salt and an amine.

DETAILED DESCRIPTION - Preparation of benzoylpyrazole derivatives of formula (I) comprises reacting a hydroxypyrazole compound of formula (II) with a bromobenzene of formula (III) in the presence of carbon monoxide, a palladium catalyst, one or more equivalents of a potassium salt and one or more equivalents of a tertiary amine of formula N(Ra)3 (IV). Reaction is at 0-40 kg/cm² and 100-140degreesC.

R1, R4 = 1-4C alkyl;

R2 = Cl or CH3;

R3 = H or 1-4C alkyl;

M = H or alkali metal;

Ra = 1-6C alkyl, or one can be phenyl or naphthyl;

the isoxazole or isoxazoline residue is bonded in the 3- or 5-position.

ACTIVITY - Herbicidal.

MECHANISM OF ACTION - None given.

USE - (I) are useful as herbicides (see WO9626206 and WO9735850).

ADVANTAGE - (I) are obtained from (II) and (III) in high yield in an economical single stage process, despite the presence of the sensitive isoxazole or isoxazoline ring. A large excess of 5-hydroxypyrazole is not required.

MANUAL CODE: CPI: C07-D08; C07-E01; C14-V01; N02-F
IN GEBHARDT J; RHEINHEIMER J; VON DEYN W; GOTZ N; HAGEN H; KEIL M;
LOCHTMAN R; RACK M; WITSCHEL M

L62 ANSWER 25 OF 25 WPIX COPYRIGHT 2009 THOMSON REUTERS on STN
ACCESSION NUMBER: 1998-378404 [33] WPIX Full-text
DOC. NO. CPI: C1998-114977 [33]
TITLE: New ((imino-methyl)benzoyl)-pyrazole derivatives -
useful as herbicides, e.g. for selective weed and weed
grass control in crops
C02; P14
DERWENT CLASS:
INVENTOR: BAUMANN E; ENGEL S; GOETZ N; GOTZ N; HILL R L; KARDOFF
U; KARDORFF U; MAYER G; MISSBLITZ U; MISSLITZ U; OTTEN
M; RACK M; REINHEIMER J; RHEINHEIMER J; VON DEYN W;
WALTER H; WESTPHALEN K; WITSCHEL M
PATENT ASSIGNEE: (BADI-C) BASF AG
COUNTRY COUNT: 49

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
DE 19700096	A1	19980709	(199833)*	DE	184	[0]
WO 9829392	A1	19980709	(199833)	DE		
AU 9860908	A	19980731	(199849)	EN		
ZA 9800007	A	19990929	(199947)	EN	290	
EP 960100	A1	19991201	(200001)	DE		
US 6028035	A	20000222	(200017)	EN		
SK 9900868	A3	20000118	(200018)	SK		
CN 1247532	A	20000315	(200031)	ZH		
BR 9714257	A	20000418	(200032)	PT		
HU 2000000491	A2	20000628	(200039)	HU		
CZ 9902393	A3	20000913	(200054)	CS		
MX 9906104	A1	19991001	(200103)	ES		
KR 2000062415	A	20001025	(200124)	KO		
JP 2001508421	W	20010626	(200140)	JA	288	
NZ 336452	A	20010629	(200140)	EN		
AU 744201	B	20020221	(200223)	EN		
IL 130600	A	20030112	(200317)	EN		
EP 960100	B1	20030709	(200353)	DE		
DE 59710430	G	20030814	(200361)	DE		
MX 207946	B	20020524	(200365)	ES		
ES 2203832	T3	20040416	(200427)	ES		
CN 1106385	C	20030423	(200538)	ZH		
SK 284921	B6	20060202	(200623)	SK		
KR 523311	B	20051024	(200680)	KO		
CZ 297520	B6	20070103	(200709)	CS		
CA 2276463	C	20070710	(200747)	EN		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 19700096	A1	DE 1997-19700096	19970103
BR 9714257	A	BR 1997-14257	19971219
CN 1247532	A	CN 1997-181884	19971219
CN 1106385	C	CN 1997-181884	19971219

DE 59710430 G
 EP 960100 A1
 EP 960100 B1
 DE 59710430 G
 ES 2203832 T3
 IL 130600 A
 NZ 336452 A
 WO 9829392 A1
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 US 6028035 A
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 BR 9714257 A
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 AU 9860908 A
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 JP 2001508421 W
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 KR 523311 B
 HU 2000000491 A2
 CA 2276463 C
 CA 2276463 C

DE 1997-510430 19971219
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 KR 1999-706036 19990702
 KR 1999-706036 19990702
 HU 2000-491 19971219
 CA 1997-2276463 19971219
 WO 1997-EP7210 19971219

FILING DETAILS:

PATENT NO	KIND		PATENT NO	
AU 744201	B	Previous Publ	AU 9860908	A
CZ 297520	B6	Previous Publ	CZ 9902393	A
DE 59710430	G	Based on	EP 960100	A
ES 2203832	T3	Based on	EP 960100	A
KR 523311	B	Previous Publ	KR 2000062415	A
SK 284921	B6	Previous Publ	SK 9900868	A
AU 9860908	A	Based on	WO 9829392	A
EP 960100	A1	Based on	WO 9829392	A
US 6028035	A	Based on	WO 9829392	A
BR 9714257	A	Based on	WO 9829392	A
HU 2000000491	A2	Based on	WO 9829392	A
CZ 9902393	A3	Based on	WO 9829392	A
KR 2000062415	A	Based on	WO 9829392	A
JP 2001508421	W	Based on	WO 9829392	A
NZ 336452	A	Based on	WO 9829392	A
AU 744201	B	Based on	WO 9829392	A

IL 130600	A	Based on	WO 9829392	A
EP 960100	B1	Based on	WO 9829392	A
DE 59710430	G	Based on	WO 9829392	A
SK 284921	B6	Based on	WO 9829392	A
KR 523311	B	Based on	WO 9829392	A
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CA 2276463	C	Based on	WO 9829392	A

PRIORITY APPLN. INFO: DE 1997-19700096 19970103
WO 1997-EP7210 19971219

INT. PATENT CLASSIF.:

MAIN: A01N0043-56; C07D231-20

IPC ORIGINAL: A01N0043-48 [I,C]; A01N0043-48 [I,C]; A01N0043-56 [I,A];
A01N0043-56 [I,A]; A01P0013-00 [I,A]; A01P0013-00 [I,C];
C07D0231-00 [I,C]; C07D0231-00 [I,C]; C07D0231-00 [I,C];
C07D0231-20 [I,A]; C07D0231-20 [I,A]; C07D0231-22 [I,A];
C07D0231-24 [I,A]; C07D0231-24 [I,C]

IPC RECLASSIF.:

A01N [I,S]; A01N0043-48 [I,C]; A01N0043-56 [I,A];
A01P0013-00 [I,C]; C07D [I,S]; C07D0231-00 [I,C];
C07D0231-00 [I,C]; C07D0231-14 [I,A]; C07D0231-20 [I,A];
C07D0231-22 [I,A]; C07D0231-24 [I,A]; C07D0409-00 [I,C];
C07D0409-10 [I,A]; C07D0409-12 [I,A]

ECLA: A01N0043-56; C07D0231-24
ICO: M07D0231:24
USCLASS NCLM: 504/282.000
NCLS: 548/365.700; 548/369.400

JAP. PATENT CLASSIF.:

MAIN/SEC.: A01N0043-56 C; A01P0013-00; C07D0231-20 B; C07D0231-20 C;
C07D0231-20 F; C07D0409-10
FTERM CLASSIF.: 4C032; 4C063; 4H011; 4C063/AA01; 4H011/AB01; 4H011/BA01;
4C063/BB07; 4H011/BB09; 4H011/BB11; 4C063/CC92;
4H011/DA15; 4H011/DA16; 4H011/DC05; 4H011/DD03;
4C063/DD22; 4C063/EE03

BASIC ABSTRACT:

DE 19700096 A1 UPAB: 20060114

4-(3-Iminomethyl-benzoyl)-pyrazole compounds of formula (I) and their salts are new. R1, R2 = H, NO2, halo, CN, rhodano, 1-6C alkyl (optionally substituted by halo or 1-6C alkoxy), 2-6C alkenyl, 2-6C alkynyl, OR5, OCOR6, OSO2R6, SH, S(O)nR7, SO2OR5, SO2NR5R8, NR8SO2R6 or NR8COR6; R3 = H, CN, 1-6C alkyl, 1-6C haloalkyl, OR7, SR7, or NR7R10; R4 = 1-6C alkyl, 3-6C cycloalkyl, 3-6C alkenyl, 4-6C cycloalkenyl, 3-6C alkynyl (all optionally substituted by Z), H, COR9, CO2R9, COSR9 or CONR8R9; X = O or NR8; n = 0-2; R5 = H, 1-6C alkyl, 1-6C haloalkyl, 1-6C alkoxy-2-6C alkyl, 3-6C alkenyl or 3-6C alkynyl; R6 = 1-6C alkyl or 1-6C haloalkyl; R7 = as for R5 but not H; R8 = H or 1-6C alkyl; R9 = 1-6C alkyl, 3-6C alkenyl, 3-6C alkynyl, phenyl or benzyl (all optionally substituted by Z); Z = 1 or more halo and/or 1-3 OH, SH, NH2, CN, R10, OR10, SR10, NR8R10, =NOR10, OCOR10, SCOR10, NR8COR10, CO2R10, COSR10, CONR8R10, 1-4C alkyliminooxy, 1-4C alkoxyamino, 1-4C alkylcarbonyl, 1-4C alkoxy-2-6C alkoxy carbonyl, 1-4C alkylsulphonyl or (all optionally substituted) heterocyclyl, heterocyclyloxy, phenyl, benzyl, heteroaryl, phenoxy, benzyloxy or heteroaryloxy; R10 = 1-6C alkyl, 1-6C haloalkyl, 3-6C alkenyl or 3-6C alkynyl; R11 = 1-6C alkyl 1-6C haloalkyl or phenyl optionally substituted by 1 or more halo and/or 1-3 substituents Z'; Z' = NO2, CN, 1-4C alkyl, 1-4C alkoxy, 1-4C haloalkyl or 1-4C haloalkoxy; R12 = 1-6C alkyl, 1-6C alkylcarbonyl or 1-6C alkylsulphonyl (all optionally substituted by halo), H, 1-6C alkoxy carbonyl, or benzoyl, methylbenzoyl, phenoxy carbonyl or phenylsulphonyl (all optionally ring-substituted by 1 or more halo and/or 1-3 substituents Z'); R13 = H, 1-6C alkyl or 1-6C haloalkyl.

USE - (I) are herbicides (claimed). They can be used to control weeds in crops such as wheat, rice maize, soya and cotton, when used in small amounts.

They can also be used for the selective pre- or post-emergence control of weeds in crops such as onion, beet, cabbage, citrus, tea, sunflower, hops, beans, sugar cane and potatoes. They may also be used to control undesired plant growth on non-cultivated areas. - Application rate is 0.001-3 kg/ha, preferably 0.01-1 kg/ha.

ADVANTAGE - (I) are more active and tolerated better by crops than the 4-benzoyl-pyrazoles known from EP 282944. MANUAL CODE: CPI: C07-D08; C14-V02; C14-V03

IN BAUMANN E; ENGEL S; GOETZ N; GÖTZ N; HILL R L; KARDOFF U; KARDORFF U;
MAYER G; MISSLITZ U; MISSLITZ U; OTTEN M; RACK M; REINHEIMER J;
RHEINHEIMER J; VON DEYN W; WALTER H; WESTPHALEN K; WITSCHEL M

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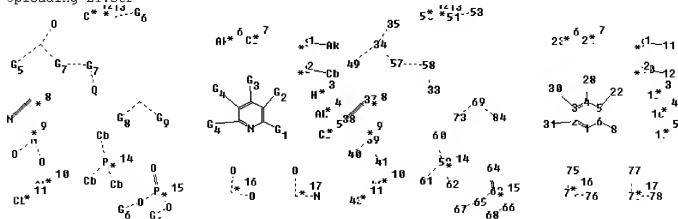
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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chain nodes :

8 9 10 11 12 15 16 17 22 23 24 28 30 31 34 35 37 38 39 40 41
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 75 76 77 78
 79 84

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

33

chain bonds :

2-31 3-30 4-28 5-22 6-8 9-11 10-12 33-58 34-49 34-35 34-57 37-38 39-40

10/584354

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69-84 74-75
74-76 77-79 78-79
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exact/norm bonds :
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51-53 57-58 59-60 59-61 59-62 63-64 63-65 63-66 65-67 66-68 69-73 69-84
74-75 74-76
77-79 78-79
exact bonds :
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normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
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G1:OH,NH2

G2:[*1],[*2],[*3],[*4],[*5]

G3:CN,NO2,[*6],[*7]

G4:H,[*6],[*7]

G5:[*8],[*9],[*10],[*11]

G6:Cb,Ak

G7:[*12],[*13]

G8:[*14],[*15]

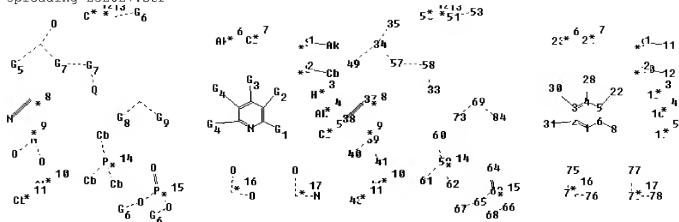
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RC ring/chain
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Match level :

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11:CLASS
12:Atom 15:CLASS 16:CLASS 17:Atom 22:CLASS 23:CLASS 24:Atom 28:CLASS
30:CLASS 31:CLASS
33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:Atom
49:CLASS 50:CLASS 51:CLASS 53:CLASS 57:CLASS 58:CLASS 59:CLASS 60:Atom
61:Atom 62:Atom
63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 73:CLASS
74:CLASS 75:CLASS
76:CLASS 77:CLASS 78:CLASS 79:CLASS 84:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 33
containing 69
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10/584354

G9:CN, [*16], [*17]

Connectivity :

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RC ring/chain 77:1 E exact RC ring/chain 78:1 E exact RC ring/chain 79:3 E exact
RC ring/chain

Match level :

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11:CLASS
12:Atom 15:CLASS 16:CLASS 17:Atom 22:CLASS 23:CLASS 24:Atom 28:CLASS
30:CLASS 31:CLASS
33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:Atom
49:CLASS 50:CLASS 51:CLASS 53:CLASS 57:CLASS 58:CLASS 59:CLASS 60:Atom
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74:CLASS 75:CLASS
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containing 1
fragments assigned reactant/reagent role:
containing 33
containing 69

=> d stat que L24

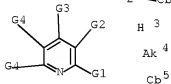
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L5 STR

Ak 6 Cb⁷



G1 OH,NH2

G2 [e1], [e2], [e3], [e4], [e5]

G3 CN,NO2, [e6], [e7]

G4 H, [e6], [e7]

Structure attributes must be viewed using STN Express query preparation.

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(O/ELS OR N>1)

10/584354

L19

STR

G1



G1 [01], [02]



Structure attributes must be viewed using STN Express query preparation.

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L22 1177 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L21

L24 2 SEA FILE=CASREACT SUB=L22 SSS FUL L1 (7 REACTIONS)

100.0% DONE 953 VERIFIED 7 HIT RXNS 2 DOCS

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L24 ANSWER 1 OF 2 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:88171 CASREACT Full-textTITLE: Process for the preparation of
4-trifluoromethyl-2(1H)-pyridinoneINVENTOR(S): Hamilton, Christopher Thomas; Gullo, Michael
Frederick; Gonzalez, Michael Allen; Roth, Gary Alan;
Gorman, David Bruce

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 9 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050288511	A1	20051229	US 2005-166485	20050624
US 7488828	B2	20090210		
WO 2006012320	A1	20060202	WO 2005-US22539	20050624
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KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

US 2004-583002P 20040625

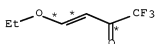
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MARPAT 144:88171

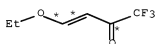
AB 4-Trifluoromethyl-2(1H)-pyridinone (I) is prepared by condensation reaction of 4-alkoxy-1,1,1-trifluorobut-3-en-2-one of formula $\text{CF}_3\text{COCH:CHOR}$ ($\text{R} = \text{C1-4 alkyl}$) or 4,4-dialkoxy-1,1,1-trifluorobutan-2-one of formula $\text{CF}_3\text{COCH}_2\text{CH(OR)}_2$ ($\text{R} = \text{same as above}$) with a trialkyl phosphonoacetate ($\text{RO})_2\text{P(O)CH}_2\text{CO}_2\text{R}$ ($\text{R} = \text{same as above}$) and cyclization of the resulting alkyl 4-(dialkoxy)-3-(trifluoromethyl)butenoate mixture of (E)- or (Z)-($\text{RO})_2\text{CHCH}_2\text{C(CF}_3\text{):CHCO}_2\text{R}$ and ($\text{RO})_2\text{CHCH:C(CF}_3\text{)CH}_2\text{CO}_2\text{R}$ ($\text{R} = \text{same as above}$). Thus, 10 g 4-ethoxy-1,1,1-trifluorobut-3-en-2-one and 15 mL ethanol were combined in a nitrogen-purged 250 mL flask in an ice bath, cooled to 10° , treated with 13.3 g tri-Et phosphonoacetate in one portion, cooled to -5° , treated with 38.6 g 21% sodium ethoxide/ethanol over 10 min while the mixture exothermed to 3.3° during the 10 min addition, slowly warmed to room temperature, stirred at room temperature overnight, and concentrated by distillation at 40° (pot temperature) under reduced pressure of 120 mmHg. After distillation, the bottoms were dissolved in 50 mL toluene then washed with water (3x40 mL) and the organic phases were combined and concentrated to give a mixture of products containing Et (E)-5,5-diethoxy-3-(trifluoromethyl)pent-2-enoate, Et (E)-5,5-diethoxy-3-(trifluoromethyl)pent-3-enoate, and Et (Z)-5,5-diethoxy-3-(trifluoromethyl)pent-2-enoate as a dark red oil (26.1 g). A distilled mixture of condensation products (5.0 g) was combined with 2.7 g ammonium acetate and 5 mL formamide in a flask equipped with a distillation head, heated in an oil bath set at $155\text{--}165^\circ$ for 2 h, treated with 0.8 g ammonium acetate, heated for another 1 h, cooled to 60° , and treated slowly with water (5 mL) and then saturated aqueous NaCl (5 mL). The resulting slurry was cooled to 15° over 1/2 h, filtered to give, after washing the product with water, 66% I. I is useful as an intermediate for herbicides.

RX(3) OF 3 COMPOSED OF RX(1), RX(2)

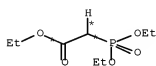
RX(3) 3 A + 3 B + 3 C ==> 3 H



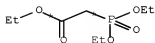
2 A



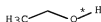
A



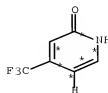
2 B

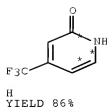
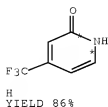


B



3 C

H
YIELD 86%



RX(1) RCT A 17129-06-5, B 867-13-0, C 141-52-6
 PRO D 872131-06-1, E 872131-07-2, F 872131-08-3
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) room temperature -> 10 deg C
 SUBSTAGE(3) -5 deg C
 SUBSTAGE(4) 0.17 hours, 3 deg C
 SUBSTAGE(5) 3 deg C -> room temperature
 SUBSTAGE(6) overnight, room temperature

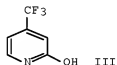
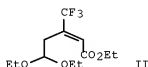
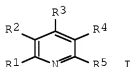
RX(2) RCT D 872131-06-1, E 872131-07-2, F 872131-08-3
 RGT I 631-61-8 NH4OAc, J 75-12-7 Formamide
 PRO H 50650-59-4
 SOL 75-12-7 Formamide
 CON 3 hours, room temperature -> 155 deg C
 NTE optimization study, thermal

L24 ANSWER 2 OF 2 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 143:133285 CASREACT Full-text
 TITLE: Process for the preparation of pyridine derivatives
 having an electron withdrawing substituent in the
 position 4 of the ring, particularly
 4-trifluoromethylpyridines
 INVENTOR(S): Gebhardt, Joachim; Goetz, Norbert; Jaedicke, Hagen;
 Mayer, Guido; Rack, Michael
 PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
 SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063780	A1	20050714	WO 2004-EP14590	20041222
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,			

	EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
AU 2004309054	A1 20050714	AU 2004-309054	20041222
CA 2550693	A1 20050714	CA 2004-2550693	20041222
EP 1723156	A1 20061122	EP 2004-804186	20041222
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
CN 1898255	A 20070117	CN 2004-80038884	20041222
BR 2004018047	A 20070417	BR 2004-18047	20041222
JP 2007519625	T 20070719	JP 2006-546051	20041222
IN 2006DN03604	A 20070824	IN 2006-DN3604	20060622
MX 2006007401	A 20060913	MX 2006-7401	20060623
KR 2006128896	A 20061214	KR 2006-712653	20060623
US 20070249837	A1 20071025	US 2007-584354	20070604
PRIORITY APPLN. INFO.:		EP 2003-29730	20031223
		US 2003-531614P	20031223
		WO 2004-EP14590	20041222

OTHER SOURCE(S): MARPAT 143:133285
GI

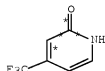
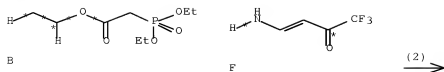


AB The invention is directed to a process for the preparation of substituted pyridine derivs. having an electron withdrawing substituent in the position 4 of the ring I [R1, R2 = independently H, (un)substituted alkyl, aryl; R3 = CN, NO2, CF3, etc.; R4 = H, (un)substituted S-alkyl, alkyl; R5 = OH, NH2] by condensation of an α - β -unsatd. carbonyl compound R3-C(O)-C(R1):C(R2)-G [R1-R3 = defined as above; G = NH2, or a leaving group] with a Wittig reagent or Horner-Wadsworth-Emmons reagent in the presence of a base, optionally followed by cyclization. For example, condensation of 4-ethoxy-1,1,1-trifluorobut-3-en-2-one with phosphonoacetic acid tri-Et ester in the presence of EtONa in EtOH, and subsequent cyclization of II with NH4OAc at 150-155 for 8 h gave pyridine III.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 26 B + F ==> G

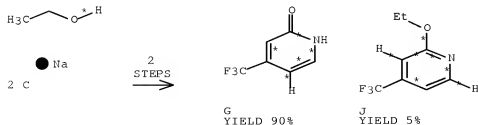
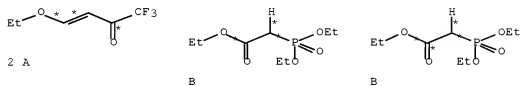
10/584354



G
YIELD 25%

RX(2) RCT B 867-13-0, F 184848-89-3
RGT H 124-41-4 NaOMe
PRO G 50650-59-4
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 10 minutes, room temperature
SUBSTAGE(2) overnight, room temperature
NTE industrial manufacture

RX(12) OF 26 COMPOSED OF RX(1), RX(3)
RX(12) 2 A + 2 B + 2 C ==> G + J



10/584354

RX(1) RCT A 17129-06-5, B 867-13-0

STAGE(1)

SOL 64-17-5 EtOH

CON 10 minutes, 10 - 13 deg C

STAGE(2)

RCT C 141-52-6

CON 25 minutes, 0 - 2 deg C

PRO D 858421-04-2

NTE Horner-Wadsworth-Emmons reagent used in first stage, mixture of isomers obtained, industrial manufacture

RX(3) RCT D 858421-04-2

STAGE(1)

RGT K 7664-41-7 NH3

SOL 7664-41-7 NH3, 109-99-9 THF, 7727-37-9 N2

CON SUBSTAGE(1) 150 minutes, 250 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT L 109-99-9 THF

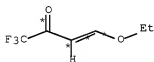
CON cooled

PRO G 50650-59-4, J 858421-08-6

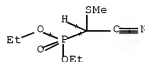
NTE gas phase, flow system, thermal, chemoselective, boron doped zeolite is used as catalyst, use of ammonium acetate gave lower yield, optimized on method of preparation, hot tube reactor used, industrial manufacture

RX(18) OF 26 COMPOSED OF RX(6), RX(7)

RX(18) A + R ==> X

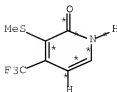


A



R

2
STEPS
→

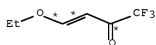


X
YIELD 77%

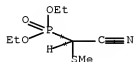
RX(6) RCT A 17129-06-5, R 858421-05-3
 RGT W 865-34-9 LiOMe
 PRO V 858421-06-4
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) 20 - 35 deg C
 SUBSTAGE(2) overnight, room temperature
 NTE stereoselective, Horner-Wadsworth-Emmons reagent used, mixture
 of E/Z isomers obtained, industrial manufacture

RX(7) RCT V 858421-06-4
 RGT Y 7664-93-9 H2SO4
 PRO X 858421-07-5
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON SUBSTAGE(1) room temperature -> 70 deg C
 SUBSTAGE(2) 5 hours, 70 deg C
 NTE chemoselective, industrial manufacture

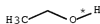
RX(19) OF 26 COMPOSED OF RX(10), RX(8)
 RX(19) 3 A + 3 R + 3 AC + I ==> X +
 AA + AB



3 A



3 R

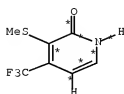


● Li
3 AC



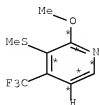
I

2
STEPS
→



X
YIELD 39%

10/584354



AA
YIELD 17%



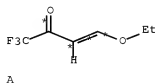
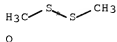
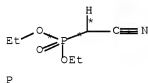
AB
YIELD 2%

RX(10) RCT A 17129-06-5, R 858421-05-3, AC 2388-07-0
 PRO Z 858421-09-7
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) 2 hours, 60 deg C
 NTE optimized on reagent, Horner-Wadsworth-Emmons reagent used,
 industrial manufacture

RX(8) RCT Z 858421-09-7, I 67-56-1
 PRO X 858421-07-5, AA 858421-10-0, AB 858421-11-1
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) 60 minutes, 230 deg C
 SUBSTAGE(2) cooled
 NTE chemoselective, thermal, boron doped zeolite is used as
 catalyst, use of ammonium acetate gave lower yield, industrial
 manufacture

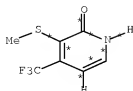
RX(23) OF 26 COMPOSED OF RX(5), RX(6), RX(7)

RX(23) P + Q + A ==> X



3
STEPS
→

10/584354



X
YIELD 77%

RX(5) RCT P 2537-48-6

STAGE(1)

RGT S 7646-69-7 NaH

SOL 109-99-9 THF

CON SUBSTAGE(1) 30 minutes, 25 - 40 deg C

SUBSTAGE(2) 30 minutes, 30 deg C

STAGE(2)

RCT Q 624-92-0

CON SUBSTAGE(1) 30 minutes, 25 deg C

SUBSTAGE(2) overnight, room temperature

STAGE(3)

RGT T 7647-01-0 HCl

SOL 7732-18-5 Water

CON 15 minutes, 25 deg C

PRO R 858421-05-3

NTE industrial manufacture

RX(6) RCT A 17129-06-5, R 858421-05-3

RGT W 865-34-9 LiOMe

PRO V 858421-06-4

SOL 67-56-1 MeOH

CON SUBSTAGE(1) 20 - 35 deg C

SUBSTAGE(2) overnight, room temperature

NTE stereoselective, Horner-Wadsworth-Emmons reagent used, mixture of E/Z isomers obtained, industrial manufacture

RX(7) RCT V 858421-06-4

RGT Y 7664-93-9 H2SO4

PRO X 858421-07-5

SOL 7732-18-5 Water, 64-17-5 EtOH

CON SUBSTAGE(1) room temperature -> 70 deg C

SUBSTAGE(2) 5 hours, 70 deg C

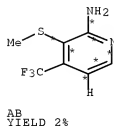
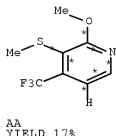
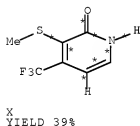
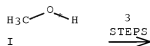
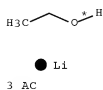
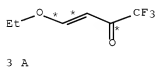
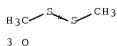
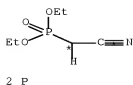
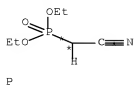
NTE chemoselective, industrial manufacture

RX(24) OF 26 COMPOSED OF RX(5), RX(10), RX(8)

RX(24) 3 P + 3 Q + 3 A + 3 AC + I ==>

X + AA + AB

10/584354



RX(5) RCT P 2537-48-6

STAGE(1)

RGT S 7646-69-7 NaH

SOL 109-99-9 THF

CON SUBSTAGE(1) 30 minutes, 25 - 40 deg C

SUBSTAGE(2) 30 minutes, 30 deg C

STAGE(2)

RCT Q 624-92-0

CON SUBSTAGE(1) 30 minutes, 25 deg C

SUBSTAGE(2) overnight, room temperature

STAGE(3)

RGT T 7647-01-0 HCl

SOL 7732-18-5 Water

CON 15 minutes, 25 deg C

PRO R 858421-05-3

NTE industrial manufacture

10/584354

RX(10) RCT A 17129-06-5, R 858421-05-3, AC 2388-07-0
PRO Z 858421-09-7
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 2 hours, 60 deg C
NTE optimized on reagent, Horner-Wadsworth-Emmons reagent used,
industrial manufacture

RX(8) RCT Z 858421-09-7, I 67-56-1
PRO X 858421-07-5, AA 858421-10-0, AB 858421-11-1
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 60 minutes, 230 deg C
SUBSTAGE(2) cooled
NTE chemoselective, thermal, boron doped zeolite is used as
catalyst, use of ammonium acetate gave lower yield, industrial
manufacture

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FILE CONTENT:1840 - 15 Mar 2009 VOL 150 ISS 12

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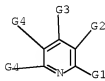
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1          STR
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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Structure attributes must be viewed using STN Express query preparation.
L5          STR
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Ak 6 Cb⁷



H 3

Ak 4

Cb 5

G1 OH,NH2
G2 [e1], [e2], [e3], [e4], [e5]
G3 CN,NO2, [e6], [e7]
G4 H, [e6], [e7]

Structure attributes must be viewed using STN Express query preparation.

10/584354

L15 3335455 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 46.156.30/RID AND
(O/ELS OR N>1)
L19 STR

G1



G1 [#1], [#2]

Structure attributes must be viewed using STN Express query preparation.

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L22 1177 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L21
L24 2 SEA FILE=CASREACT SUB=L22 SSS FUL L1 (7 REACTIONS)
L37 4 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON ("134:193342"/AN OR
"143:133285"/AN OR "144:88171"/AN OR "150:98169"/AN OR
"2001:170612"/AN OR "2005:1346086"/AN OR "2005:612313"/AN OR
"2009:3706"/AN)
L38 8 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON 50650-59-4
L39 4 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L37 AND L38
L40 2 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L39 NOT L24

=> d ibib abs hit L40 1-2

L40 ANSWER 1 OF 2 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 150:98169 CASREACT Full-text
TITLE: Process for the preparation of
4-trifluoromethyl-2(1H)-pyridinone
INVENTOR(S): Bland, Douglas C.; Davies, John
PATENT ASSIGNEE(S): Dow AgroSciences LLS, USA
SOURCE: U.S. Pat. Appl. Publ., 9pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090005569	A1	20090101	US 2008-147973	20080627
WO 2009006211	A1	20090108	WO 2008-US68368	20080626

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK,

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TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
 TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
 AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

US 2007-937799P 20070629

OTHER SOURCE(S):

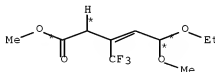
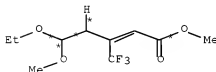
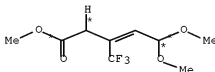
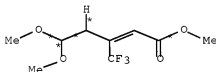
MARPAT 150:98169

GI



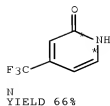
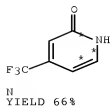
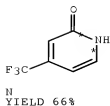
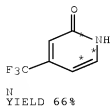
AB 4-Trifluoromethyl-2(1H)-pyridinone (I) is prepared from an alkyl vinyl ether, $\text{H}_2\text{C}:\text{CHCH}_2\text{OR}$ [$\text{R} = \text{C1-4-alkyl}$] and trifluoroacetyl chloride in a four step process. The process comprises: (i) contacting $\text{H}_2\text{C}:\text{CHCH}_2\text{OR}$ with $\text{ClC}(\text{:O})\text{CF}_3$ to provide 4-chloro-4-alkoxy-1,1,1-trifluoro-2-butanone, $\text{CF}_3\text{C}(\text{:O})\text{CH}_2\text{CHClOR}$; (ii) contacting the butanone with a C1-4-alc. to provide a mixture of acetals, $\text{CF}_3\text{C}(\text{:O})\text{CH}_2\text{CH}(\text{OR})_2$ and $\text{CF}_3\text{C}(\text{OH})(\text{OR})\text{CH}_2\text{CH}(\text{OR})_2$; (iii) contacting the acetals with trialkyl phosphonoacetate, $(\text{RO})_2\text{P}(\text{:O})\text{CH}_2\text{CO}_2\text{R}$, in the presence of a base and an alc. or glycol solvent to provide a mixture of alkenoates, $\text{RO}_2\text{CCH}:\text{C}(\text{CF}_3)\text{CH}_2\text{CH}(\text{OR})_2$ and $\text{RO}_2\text{CCH}_2\text{C}(\text{CF}_3):\text{CHCH}(\text{OR})_2$; and, (iv) cyclizing the alkenoates to provide I.

RX(5) OF 12 ...I + J + K + L ==> 4 N



(5) →

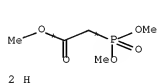
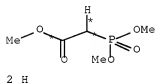
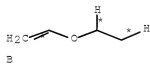
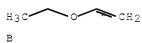
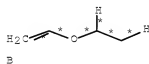
10/584354



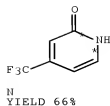
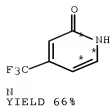
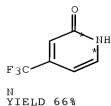
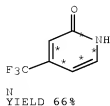
RX(5) RCT I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4
 RGT O 631-61-8 NH4OAc, P 75-12-7 Formamide
 PRO N 50650-59-4
 CON SUBSTAGE(1) room temperature -> 140 deg C
 SUBSTAGE(2) 13 minutes, >130 deg C
 SUBSTAGE(4) 3.25 hours

RX(8) OF 12 COMPOSED OF RX(3), RX(5)

RX(8) 4 A + 4 B + 4 D + 4 H ==> 4 N



2
STEPS
→



RX(3) RCT A 354-32-5, B 109-92-2

STAGE(1)

SOL 109-92-2 EtOCH:CH2
CON SUBSTAGE(1) cooled
SUBSTAGE(2) room temperature
SUBSTAGE(3) 30 minutes, room temperature

STAGE(2)

RCT D 67-56-1
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 24 minutes, cooled
SUBSTAGE(2) 1 hour
SUBSTAGE(3) overnight
SUBSTAGE(4) cooled

STAGE(3)

RCT H 5927-18-4
RGT M 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON SUBSTAGE(1) cooled
SUBSTAGE(2) 9 minutes, cooled
SUBSTAGE(3) room temperature
SUBSTAGE(4) 1 hour

PRO I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4

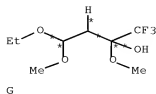
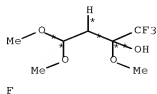
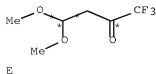
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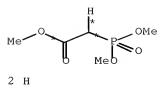
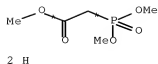
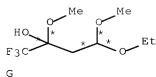
RGT O 631-61-8 NH4OAc, P 75-12-7 Formamide
PRO N 50650-59-4

CON SUBSTAGE(1) room temperature -> 140 deg C
SUBSTAGE(2) 13 minutes, >130 deg C
SUBSTAGE(4) 3.25 hours

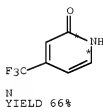
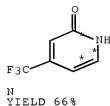
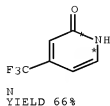
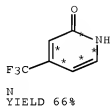
RX(9) OF 12 COMPOSED OF RX(4), RX(5)

RX(9) E + F + 2 G + 4 H ==> 4 N





2
STEPS
→



RX(4) RCT E 1095142-51-0, F 1095142-53-2, G 1095142-55-4

STAGE(1)

RGT M 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON <20 deg C, basify

STAGE(2)

RCT H 5927-18-4
RGT M 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON SUBSTAGE(2) 2 deg C
SUBSTAGE(3) 15 minutes, 2 deg C -> 8 deg C
SUBSTAGE(4) 2.5 hours, 8 deg C -> room temperature

PRO I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4

RX(5) RCT I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4
RGT O 631-61-8 NH4OAc, P 75-12-7 Formamide

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PRO N 50650-59-4

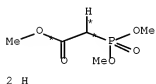
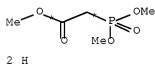
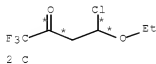
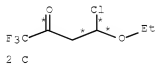
CON SUBSTAGE(1) room temperature -> 140 deg C

SUBSTAGE(2) 13 minutes, >130 deg C

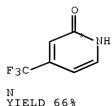
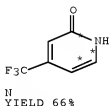
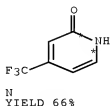
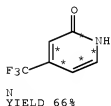
SUBSTAGE(4) 3.25 hours

RX(11) OF 12 COMPOSED OF RX(2), RX(4), RX(5)

RX(11) 4 C + 9 D + 4 H ==> 4 N



3
STEPS
→



RX(2) RCT C 1095142-49-6, D 67-56-1

PRO E 1095142-51-0, F 1095142-53-2, G 1095142-55-4

SOL 67-56-1 MeOH

CON 20 minutes, <15 deg C

RX(4) RCT E 1095142-51-0, F 1095142-53-2, G 1095142-55-4

STAGE(1)

RGT M 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON <20 deg C, basify

STAGE(2)

RCT H 5927-18-4

RGT M 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON SUBSTAGE(2) 2 deg C

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PRO E 1095142-51-0, F 1095142-53-2, G 1095142-55-4
 SOL 67-56-1 MeOH
 CON 20 minutes, <15 deg C

RX(4) RCT E 1095142-51-0, F 1095142-53-2, G 1095142-55-4

STAGE(1)
 RGT M 124-41-4 NaOMe
 SOL 67-56-1 MeOH
 CON <20 deg C, basify

STAGE(2)
 RCT H 5927-18-4
 RGT M 124-41-4 NaOMe
 SOL 67-56-1 MeOH
 CON SUBSTAGE(2) 2 deg C
 SUBSTAGE(3) 15 minutes, 2 deg C -> 8 deg C
 SUBSTAGE(4) 2.5 hours, 8 deg C -> room temperature

PRO I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4

RX(5) RCT I 1095142-57-6, J 1095142-59-8, K 1095142-61-2, L 1095142-63-4
 RGT O 631-61-8 NH4OAc, P 75-12-7 Formamide
 PRO N 50650-59-4
 CON SUBSTAGE(1) room temperature -> 140 deg C
 SUBSTAGE(2) 13 minutes, >130 deg C
 SUBSTAGE(4) 3.25 hours

AN 150:98169 CASREACT Full-text

L40 ANSWER 2 OF 2 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:193342 CASREACT Full-text

TITLE: Method for synthesizing 4-trifluoromethyl pyridine compounds

INVENTOR(S): Jiang, Biao; Zhang, Fangjiang; Si, Yugui; Xiong, Wennan; Tan, Longquan

PATENT ASSIGNEE(S): Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.
 CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

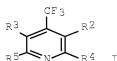
PATENT INFORMATION:

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CN 1103757	C	20030326		

PRIORITY APPLN. INFO.: CN 1999-127004 19991229

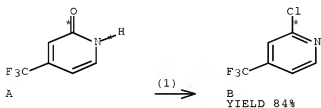
OTHER SOURCE(S): MARPAT 134:193342

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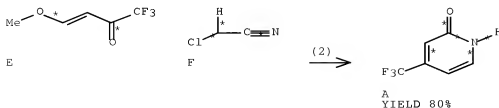
AB Title compds. {I; R1 = H, C1-4 alkyl; R2 = H, CH3, CH3CH2, C6H5, aromatic heterocyclyl; R3 = H, C1-4 alkyl, aryl, aromatic heterocyclyl; R4, R5 independently = H, C1-4 alkoxy, OH, SH, X; X = Cl, Br, I} are prepared by adding CF3COC(R3):CHOR1 with R2CHXCN in aprotic solvent in the presence of metal (Zn, Mg, Zn-Ag, Zn-Cu) and trialkylhalosilane ((CH3)3SiCl, (CH3)3SiBr, (CH3CH2)3SiCl, (CH3CH2)3SiBr); at 50-80°, and cyclizing with PX5 (PCl5, PBr5) or HCl in organic solvent. The mole ratio of butene ketone-acetonitrile-metal- trialkylhalosilane is 1:1-2:1-2:0.005-0.02. The metal is Zn, Mg, Zn/Ag, or Zn/Cu. The aprotic solvent is DMSO, THF, HMPA, DMF, benzene, toluene, or xylene. The organic solvent is dichloromethane, chloroform, CCl4, or DMF. Thus, the title compound I (R2 = H; R3 = H; R4 = H; R5 = OH) was prepared with 80% yield.

RX(1) OF 3 ...A ==> B



RX(1) RCT A 50650-59-4
RGT C 10026-13-8 PCl5
PRO B 81565-18-6
SOL 68-12-2 DMF

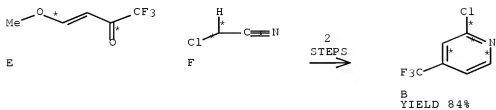
RX(2) OF 3 E + F ==> A...



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RX(2) RCT E 326894-81-9, F 107-14-2
 RGT G 7440-66-6 Zn, H 75-77-4 Me3SiCl
 PRO A 50650-59-4
 SOL 109-99-9 THF

RX(3) OF 3 COMPOSED OF RX(2), RX(1)
 RX(3) E + F ==> B



RX(2) RCT E 326894-81-9, F 107-14-2
 RGT G 7440-66-6 Zn, H 75-77-4 Me3SiCl
 PRO A 50650-59-4
 SOL 109-99-9 THF

RX(1) RCT A 50650-59-4
 RGT C 10026-13-8 PC15
 PRO B 81565-18-6
 SOL 68-12-2 DMF

AN 134:193342 CASREACT [Full-text](#)

=> d his full

(FILE 'HOME' ENTERED AT 09:30:00 ON 18 MAR 2009)

FILE 'CASREACT' ENTERED AT 09:30:09 ON 18 MAR 2009

L1 STRUCTURE UPLOADED
 L2 0 SEA SSS SAM L1 (0 REACTIONS)

FILE 'CAPLUS' ENTERED AT 09:31:13 ON 18 MAR 2009

E US2007-584354/APPS
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 D SCA
 SEL RN

FILE 'REGISTRY' ENTERED AT 09:32:19 ON 18 MAR 2009

L4 15 SEA SPE=ON ABB=ON PLU=ON (17129-06-5/BI OR 184848-89-3/BI
 OR 2537-48-6/BI OR 50650-59-4/BI OR 7664-41-7/BI OR 858421-04-2
 /BI OR 858421-05-3/BI OR 858421-06-4/BI OR 858421-07-5/BI OR
 858421-08-6/BI OR 858421-09-7/BI OR 858421-10-0/BI OR 858421-11
 -1/BI OR 858421-12-2/BI OR 867-13-0/BI)
 D SCA

FILE 'REGISTRY' ENTERED AT 09:41:06 ON 18 MAR 2009

L5 STRUCTURE UPLOADED
 L6 STRUCTURE UPLOADED
 L7 STRUCTURE UPLOADED
 L8 10 SEA SSS SAM L5
 D SCA
 L9 2 SEA SPE=ON ABB=ON PLU=ON L8 AND OXO/CNS
 D SCA
 D RSD 1
 L10 10 SEA SPE=ON ABB=ON PLU=ON 46.156.30/RID AND L8
 L11 8 SEA SPE=ON ABB=ON PLU=ON L10 NOT L9
 L12 1 SEA SPE=ON ABB=ON PLU=ON L11 AND 33/C
 D RN
 L13 STR 634910-34-2
 D
 D SCA L11
 L14 4319 SEA SPE=ON ABB=ON PLU=ON 2-HYDROXY/CNS (2W) ?PYRID?/CNS
 L15 3335455 SEA SPE=ON ABB=ON PLU=ON 46.156.30/RID AND (O/ELS OR N>1)
 L16 4 SEA SUB=L15 SSS SAM L5
 L*** DEL STRUCTURE UPLOADED
 L17 STRUCTURE UPLOADED
 L18 4 SEA SUB=L15 SSS SAM L5 AND L17
 L19 STRUCTURE UPLOADED
 L20 4 SEA SUB=L15 SSS SAM L5 AND L19
 D SCA

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FILE 'REGISTRY' ENTERED AT 10:03:15 ON 18 MAR 2009

D STAT QUE L20
 L21 12894 SEA SUB=L15 SSS FUL L5 AND L19
 SAVE CHA354L5L19/A L21

FILE 'CASREACT' ENTERED AT 10:06:18 ON 18 MAR 2009

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10/584354

L24 2 SEA SUB=L22 SSS FUL L1 (7 REACTIONS)
D SCA
SEL RX

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/RN OR 624-92-0/RN OR 75-12-7/RN OR 7646-69-7/RN OR 7647-01-0/R
N OR 7664-41-7/RN OR 7664-93-9/RN OR 858421-04-2/RN OR
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D RN
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L29 1 SEA SUB=L21 FAM FUL L28
L30 D SCA

FILE 'ZCAPLUS' ENTERED AT 10:12:01 ON 18 MAR 2009

L31 27 SEA SPE=ON ABB=ON PLU=ON L30
L32 8 SEA SPE=ON ABB=ON PLU=ON L30 (L) PREP/RL
SEL RN

FILE 'REGISTRY' ENTERED AT 10:12:29 ON 18 MAR 2009

L33 204 SEA SPE=ON ABB=ON PLU=ON (50650-59-4/BI OR 81565-18-6/BI OR
17129-06-5/BI OR 39890-98-7/BI OR 106447-97-6/BI OR 107-14-2/BI
OR 107-91-5/BI OR 121307-79-7/BI OR 24057-28-1/BI OR 356518-29
-1/BI OR 540-69-2/BI OR 631-61-8/BI OR 75-12-7/BI OR 75-90-1/BI
OR 7664-41-7/BI OR 867-13-0/BI OR 104040-74-6/BI OR 106-95-6/B
I OR 107734-26-9/BI OR 108-88-3/BI OR 109-01-3/BI OR 109-92-2/B
I OR 109-99-9/BI OR 1095142-49-6/BI OR 1095142-51-0/BI OR
1095142-53-2/BI OR 1095142-55-4/BI OR 1095142-57-6/BI OR
1095142-59-8/BI OR 1095142-61-2/BI OR 1095142-63-4/BI OR
109919-31-5/BI OR 110-89-4/BI OR 110-91-8/BI OR 1112-48-7/BI
OR 114892-27-2/BI OR 118078-66-3/BI OR 120407-73-0/BI OR
132664-24-5/BI OR 1330-20-7/BI OR 13600-42-5/BI OR 139717-71-8/
BI OR 141-52-6/BI OR 149108-61-2/BI OR 149108-62-3/BI OR
1520-70-3/BI OR 1617-17-0/BI OR 175205-81-9/BI OR 183610-70-0/B
I OR 184848-89-3/BI OR 189265-99-4/BI OR 19481-82-4/BI OR
2028-63-9/BI OR 211098-45-2/BI OR 219986-54-6/BI OR 220459-51-8
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220459-55-2/BI OR 220459-56-3/BI OR 220459-58-5/BI OR 220459-59
-6/BI OR 220459-60-9/BI OR 220459-61-0/BI OR 220459-62-1/BI OR
22245-83-6/BI OR 22253-59-4/BI OR 2537-48-6/BI OR 2857-97-8/BI
OR 289503-26-0/BI OR 31271-90-6/BI OR 326894-65-9/BI OR
326894-66-0/BI OR 326894-67-1/BI OR 326894-68-2/BI OR 326894-69
-3/BI OR 326894-70-6/BI OR 326894-71-7/BI OR 326894-72-8/BI OR
326894-73-9/BI OR 326894-74-0/BI OR 326894-75-1/BI OR 326894-76
-2/BI OR 326894-77-3/BI OR 326894-78-4/BI OR 326894-79-5/BI OR
326894-80-8/BI OR 326894-81-9/BI OR 326894-82-0/BI OR 326894-83
-1/BI OR 326922-19-4/BI OR 326922-20-7/BI OR 326922-21-8/BI OR
326922-22-9/BI OR 326922-23-0/BI OR 326922-24-1/BI OR 326922-25
-2/BI OR 326922-26-3/BI OR 326922-27-4/BI OR 339539-96-7/BI OR

```

339539-98-9/BI OR 339539-99-0/BI
L34      5 SEA SPE=ON ABB=ON PLU=ON L33 AND P/ELS
          D SCA

FILE 'ZCAPLUS' ENTERED AT 10:13:16 ON 18 MAR 2009
L35      4 SEA SPE=ON ABB=ON PLU=ON L32 AND L34
          D SCA
L36      4 SEA SPE=ON ABB=ON PLU=ON L35 AND CASREACT/OS
          SEL AN

FILE 'CASREACT' ENTERED AT 10:15:37 ON 18 MAR 2009
L37      4 SEA SPE=ON ABB=ON PLU=ON ("134:193342"/AN OR "143:133285"/AN
          OR "144:88171"/AN OR "150:98169"/AN OR "2001:170612"/AN OR
          "2005:1346086"/AN OR "2005:612313"/AN OR "2009:3706"/AN)
L38      8 SEA SPE=ON ABB=ON PLU=ON 50650-59-4
L39      4 SEA SPE=ON ABB=ON PLU=ON L37 AND L38
          D OCC 1-
          D HIT 1-4

FILE 'CASREACT' ENTERED AT 10:17:00 ON 18 MAR 2009
          D COST FUL
L40      2 SEA SPE=ON ABB=ON PLU=ON L39 NOT L24
          D HIT 1-2

FILE 'STNGUIDE' ENTERED AT 10:23:45 ON 18 MAR 2009

FILE 'CAPLUS' ENTERED AT 10:29:52 ON 18 MAR 2009
L41      178 SEA SPE=ON ABB=ON PLU=ON GEBHARDT J7/AU
L42      57 SEA SPE=ON ABB=ON PLU=ON GOTZ N7/AU
L43      43 SEA SPE=ON ABB=ON PLU=ON JAEDICKE H7/AU
L44      1001 SEA SPE=ON ABB=ON PLU=ON MAYER G7/AU
L45      210 SEA SPE=ON ABB=ON PLU=ON RACK M7/AU
L46      17 SEA SPE=ON ABB=ON PLU=ON L41 AND (L42 OR L43 OR L44 OR L45)

L47      26 SEA SPE=ON ABB=ON PLU=ON L42 AND (L43 OR L44 OR L45)
L48      1 SEA SPE=ON ABB=ON PLU=ON L43 AND (L44 OR L45)
L49      13 SEA SPE=ON ABB=ON PLU=ON L44 AND L45
L50      47 SEA SPE=ON ABB=ON PLU=ON (L46 OR L47 OR L48 OR L49)
L51      7 SEA SPE=ON ABB=ON PLU=ON L50 AND ?PYRIDIN?/AB
L52      32 SEA SPE=ON ABB=ON PLU=ON (L41 OR L42 OR L43 OR L44 OR L45)
          AND ?PYRIDIN?/AB
L53      2 SEA SPE=ON ABB=ON PLU=ON L52 AND ?PHOSPH?/AB
          D HIT 1-2
L54      6 SEA SPE=ON ABB=ON PLU=ON L46 AND (L47 OR L48 OR L49)
L55      3 SEA SPE=ON ABB=ON PLU=ON L47 AND (L48 OR L49)
L56      1 SEA SPE=ON ABB=ON PLU=ON L48 AND L49
L57      8 SEA SPE=ON ABB=ON PLU=ON (L54 OR L55 OR L56)

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:34:23 ON 18 MAR 2009
L58      7 SEA SPE=ON ABB=ON PLU=ON L53
L59      19 SEA SPE=ON ABB=ON PLU=ON L57

FILE 'CAPLUS' ENTERED AT 10:35:56 ON 18 MAR 2009
          D STAT QUE L53
          D STAT QUE L57
L60      9 SEA SPE=ON ABB=ON PLU=ON L53 OR L57

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:36:16 ON 18 MAR 2009
          D STAT QUE L58
          D STAT QUE L59

```

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L61      25 SEA SPE=ON  ABB=ON  PLU=ON  L58 OR L59

      FILE 'CAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:36:39 ON 18
      MAR 2009
L62      25 DUP REM L60 L61 (9 DUPLICATES REMOVED)
           ANSWERS '1-9' FROM FILE CAPLUS
           ANSWERS '10-17' FROM FILE BIOSIS
           ANSWERS '18-25' FROM FILE WPIX
      D IBIB ABS HITIND L62 1-9
      D IALL L62 10-17
      D IALL HIT L62 18-25

      FILE 'CASREACT' ENTERED AT 10:38:30 ON 18 MAR 2009
           D STAT QUE L24
           D IBIB ABS HIT L24 1-2

      FILE 'CASREACT' ENTERED AT 10:39:11 ON 18 MAR 2009
           D STAT QUE L40
           D IBIB ABS HIT L40 1-2

```

FILE HOME

FILE CASREACT

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FILE CONTENT:1840 - 15 Mar 2009 VOL 150 ISS 12

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*
*      CASREACT now has more than 16.5 million reactions      *
*

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STRUCTURE FILE UPDATES: 16 MAR 2009 HIGHEST RN 1122148-13-3
DICTIONARY FILE UPDATES: 16 MAR 2009 HIGHEST RN 1122148-13-3

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<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 13, 2009 (20090313/UP).

FILE ZCAPLUS

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FILE MEDLINE

FILE LAST UPDATED: 15 Mar 2009 (20090315/UP). FILE COVERS 1949 TO DATE.

MEDLINE and LMEEDLINE have been updated with the 2009 Medical Subject Headings (MeSH) vocabulary and tree numbers from the U.S. National Library of Medicine (NLM). Additional information is available at

http://www.nlm.nih.gov/pubs/techbull/nd08/nd08_medline_data_changes_2009.

On February 21, 2009, MEDLINE was reloaded. See HELP RLOAD for details.

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See HELP RANGE before carrying out any RANGE search.

FILE EMBASE

FILE COVERS 1974 TO 18 Mar 2009 (20090318/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 11 March 2009 (20090311/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED: 13 MAR 2009 <20090313/UP>

MOST RECENT UPDATE: 200916 <200916/DW>

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>>> IPC and US National Classifications have been updated with reclassifications to the end of 2008.
ECLA, F-Term and FI-Term classifications are complete to the end of 2008.

No update date (UP) has been created for the reclassified documents, but they can be identified by specific update codes (see HELP CLA for details)<<<

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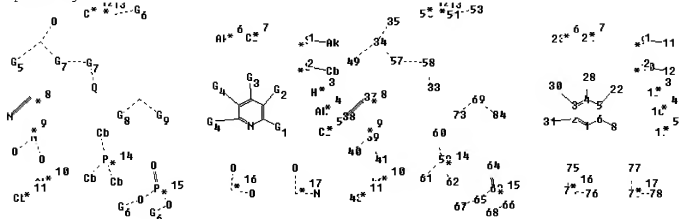
<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate>

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http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

Uploading L1.str



chain nodes :

8 9 10 11 12 15 16 17 22 23 24 28 30 31 34 35 37 38 39 40 41
42 43 49 50 51 53 57 58 59 60 61 62 63 64 65 66 67 68 69 73 74
75 76 77 78
79 84

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

33

chain bonds :

2-31 3-30 4-28 5-22 6-8 9-11 10-12 33-58 34-49 34-35 34-57 37-38 39-40
39-41 51-53 57-58 59-60 59-61 59-62 63-64 63-65 63-66 65-67 66-68 69-73
69-84 74-75
74-76 77-79 78-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-31 3-30 4-28 5-22 6-8 9-11 33-58 34-49 34-35 34-57 37-38 39-40 39-41
51-53 57-58 59-60 59-61 59-62 63-64 63-65 63-66 65-67 66-68 69-73 69-84
74-75 74-76
77-79 78-79

exact bonds :

10-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

10/584354

G1:OH,NH2

G2:[*1],[*2],[*3],[*4],[*5]

G3:CN,NO2,[*6],[*7]

G4:H,[*6],[*7]

G5:[*8],[*9],[*10],[*11]

G6:Cb,Ak

G7:[*12],[*13]

G8:[*14],[*15]

G9:CN,[*16],[*17]

Connectivity :

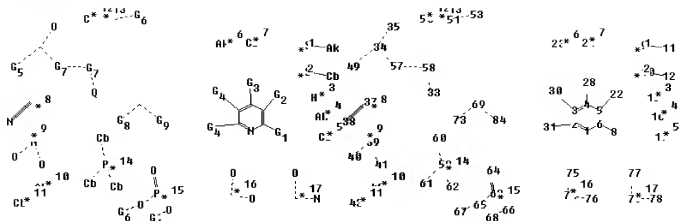
34:3 E exact RC ring/chain 35:1 E exact RC ring/chain 39:3 E exact RC ring/chain
50:2 E exact RC ring/chain 51:3 E exact RC ring/chain 74:3 E exact RC ring/chain
75:1 E exact
RC ring/chain 77:1 E exact RC ring/chain 78:1 E exact RC ring/chain 79:3 E exact
RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS
12:Atom 15:CLASS 16:CLASS 17:Atom 22:CLASS 23:CLASS 24:Atom 28:CLASS
30:CLASS 31:CLASS
33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:Atom
49:CLASS 50:CLASS 51:CLASS 53:CLASS 57:CLASS 58:CLASS 59:CLASS 60:Atom
61:Atom 62:Atom
63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 73:CLASS
74:CLASS 75:CLASS
76:CLASS 77:CLASS 78:CLASS 79:CLASS 84:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 33
containing 69

Uploading L5L6L7.str

10/584354



chain nodes :

8 9 10 11 12 15 16 17 22 23 24 28 30 31 34 35 37 38 39 40 41
42 43 49 50 51 53 57 58 59 60 61 62 63 64 65 66 67 68 69 73 74
75 76 77 78
79 84

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

33

chain bonds :

2-31 3-30 4-28 5-22 6-8 9-11 10-12 33-58 34-49 34-35 34-57 37-38 39-40
39-41 51-53 57-58 59-60 59-61 59-62 63-64 63-65 63-66 65-67 66-68 69-73
69-84 74-75
74-76 77-79 78-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-31 3-30 4-28 5-22 6-8 9-11 33-58 34-49 34-35 34-57 37-38 39-40 39-41
51-53 57-58 59-60 59-61 59-62 63-64 63-65 63-66 65-67 66-68 69-73 69-84
74-75 74-76
77-79 78-79

exact bonds :

10-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:OH,NH2

G2:[*1],[*2],[*3],[*4],[*5]

G3:CN,NO2,[*6],[*7]

G4:H,[*6],[*7]

G5:[*8],[*9],[*10],[*11]

G6:Cb,Ak

G7:[*12],[*13]

G8:[*14],[*15]

G9:CN,[*16],[*17]

Connectivity :

34:3 E exact RC ring/chain 35:1 E exact RC ring/chain 39:3 E exact RC ring/chain
 50:2 E exact RC ring/chain 51:3 E exact RC ring/chain 74:3 E exact RC ring/chain
 75:1 E exact
 RC ring/chain 77:1 E exact RC ring/chain 78:1 E exact RC ring/chain 79:3 E exact
 RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
 11:CLASS
 12:Atom 15:CLASS 16:CLASS 17:Atom 22:CLASS 23:CLASS 24:Atom 28:CLASS
 30:CLASS 31:CLASS
 33:CLASS 34:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS
 42:CLASS 43:Atom
 49:CLASS 50:CLASS 51:CLASS 53:CLASS 57:CLASS 58:CLASS 59:CLASS 60:Atom
 61:Atom 62:Atom
 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 73:CLASS
 74:CLASS 75:CLASS
 76:CLASS 77:CLASS 78:CLASS 79:CLASS 84:CLASS
 fragments assigned product role:
 containing 1
 fragments assigned reactant/reagent role:
 containing 33
 containing 69

=>